The Perturbed Static Path Approximation at Finite Temperature: Observables and Strength Functions

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Abstract

We present an approximation scheme for calculating observables and strength functions of finite fermionic systems at finite temperature such as hot nuclei. The approach is formulated within the framework of the Hubbard-Stratonovich transformation and goes beyond the static path approximation and the RPA by taking into account small amplitude time-dependent fluctuations around each static value of the auxiliary fields. We show that this perturbed static path approach can be used systematically to obtain good approximations for observable expectation values and for low moments of the strength function. The approximation for the strength function itself, extracted by an analytic continuation from the imaginary-time response function, is not always reliable, and we discuss the origin of the discrepancies and possible improvements. Our results are tested in a solvable many-body model.

I. INTRODUCTION

Mean-field approximations [1,2], such as the finite temperature Hartree-Fock (HF), are standard for describing nuclei at finite temperature. Collective excitations of the system are obtained by linearizing the time-dependent HF equations around the static HF solution, leading to the finite temperature random phase approximation (RPA) [3]. However, this treatment is inadequate for situations where various nuclear configurations compete and have comparable free energies, which causes observables to fluctuate widely about their mean values. This is the case, for example, in the vicinity of a shape transition from a spherical to a deformed nucleus, where various discontinuities predicted in the mean-field approach are smoothed in the finite nuclear system by the presence of fluctuations. Large fluctuations in the nuclear shape also play an important role in giant dipole resonances (GDR) whose frequency is strongly coupled to the quadrupole deformation. In the adiabatic approximation, the observed GDR strength function is obtained by integrating the strength function that corresponds to each quadrupole configuration over all possible configurations weighted by their respective Boltzmann factor [4].

It has been shown [2,5] that a systematic description of fluctuations can be obtained in the framework of the auxiliary-field path integral (Hubbard-Stratonovich transformation [6]). In this framework the original many-body propagator (in imaginary time) is decomposed into a superposition of one-body propagators describing non-interacting fermions moving in a fluctuating external time-dependent potential (auxiliary fields). The expectation value of any observable is represented as a weighted average of its expectation values in the corresponding non-interacting systems. Applying the method of steepest descent one can obtain self-consistent mean-field approximations at finite temperature. By taking into account small amplitude time-dependent fluctuations of the auxiliary fields around the mean-field solution in the Gaussian approximation one rederives the RPA [5,7].

The path integral representation also constitutes a starting point for exact numerical solution of the many-body problem where the auxiliary field integration is performed by Monte Carlo techniques that were recently developed for strongly correlated electron systems [8] and for the interacting nuclear shell model [9]. In the latter case a practical solution to the Monte Carlo sign problem [10], which is generic to all fermionic systems, enables the study of nuclear properties in medium and heavy mass nuclei using realistic effective interactions. The auxiliary field formulation also suggests new approximation schemes which are non-perturbative, the simplest of which is the static path approximation (SPA) [11] – [17]. Here, the path integral is approximated by summing over the time-independent fields only, weighted by the appropriate Boltzmann factor. This amounts to averaging over all possible static mean-field configurations rather than the self-consistent ones alone. The SPA has been used to calculate free energies and level densities in nuclei and was found to be superior to the mean-field approximation. In particular, it accounts for the enhancement of level density due to thermal fluctuations of the shape [13]. More recently the approximation has also been applied to the calculation of strength functions [16]. At high temperatures the SPA partition function approaches the exact result. However, as the temperature decreases the SPA becomes inaccurate since time-dependent fluctuations about the mean-field configurations can no longer be neglected. This is manifested especially in the strength function where even its first moment is significantly underestimated [16].

Recently, a method to improve the SPA has been proposed for the partition function [18–21]. In this approach contributions from time-dependent fields in the neighborhood of each static field are incorporated perturbatively to the second order in their amplitudes. When one considers such time-dependent fluctuations around the equilibrium configuration only, one obtains the RPA corrections to the partition function. However, in the proposed approach such small amplitude time-dependent fluctuations are taken around each static configuration of the auxiliary fields and the static integration is still fully retained. At even lower temperatures some of these time-dependent fluctuations can become unstable and the approximation breaks down. However, this happens only at temperatures below the phase transition, when the temperature drops below the largest imaginary RPA frequency. We remark that as a saddle point develops in the nuclear free energy surface below the transition temperature, it is still possible that the imaginary RPA frequencies are small enough in magnitude that the time-dependent fluctuations are all stable (although there is an unstable direction in the static free energy surface). This approximation scheme has been applied to free energy and level density calculations in simple models and shown to work well down to low temperatures.

It is interesting to investigate whether incorporating small time-dependent fluctuations provides a significant improvement over the SPA evaluation of quantities other than the partition function. This paper will explore the validity and applicability of this scheme, which we term the perturbed static-path approximation (PSPA), for the calculation of expectation values of observables at finite temperature as well as of strength functions. Previous work employed a formulation of the PSPA based on ordinary quantum-mechanical perturbation theory [19,20], which was specialized for free energy calculations and is not easily extended to other quantities. We therefore reformulate it in a general way, using many-body methods, and apply it to the calculation of observables and strength functions. By testing the PSPA in a solvable model we find that the PSPA results agree closely with the exact solution for observable expectation values and for low moments of the strength function. The strength function itself is approximated well at high temperatures and also at low temperatures for a certain regime of the model's parameters, although the low-temperature results generally do not improve much on the SPA. We discuss possible improvements.

This paper is organized as follows. In Section II we review the auxiliary-field path integral formalism and in Section III we formulate the PSPA for the partition function. Section IV discusses the application of the PSPA to the calculation of expectation values of one- and two-body operators. Finally, in Section V we present a treatment of the strength function and its lowest two moments in this framework. We illustrate the PSPA and compare it to other approximations in a simple model whose exact solution is given in Appendix B.

II. AUXILIARY FIELD PATH INTEGRAL

In this Section we briefly review the auxiliary-field path integral representation of the imaginary-time evolution operator for an Hamiltonian with two-body interactions (Hubbard-Stratonovich transformation) [2,5]. We consider a system of interacting fermions, and assume for simplicity an Hamiltonian of the form

$$H = K - \frac{1}{2}\chi V^2 \ , \tag{1}$$

where K and V are one-body operators

$$K = \sum_{ij} k_{ij} a_i^\dagger a_j \ , \qquad V = \sum_{ij} v_{ij} a_i^\dagger a_j \ . \tag{2}$$

$a_i^\dagger$, a_i are creation and annihilation operators for a set of single particle states i, and χ is a coupling constant. Our results can be easily generalized to a superposition of such separable interactions

$$H = K - \frac{1}{2}\sum_{\alpha=1}^{q} \chi_\alpha V_\alpha^2 \ . \tag{3}$$

We remark that an arbitrary two-body interaction

$$\begin{aligned}\sum_{ijkl} u_{ijkl} a_i^\dagger a_j^\dagger a_l a_k &= \sum_{ij}\left(\sum_k u_{ikjk}\right) a_i^\dagger a_j - \sum_{ijkl} u_{iklj} a_i^\dagger a_j a_k^\dagger a_l \\ &\equiv \sum_{\alpha=1}^{q} \tilde{u}_\alpha \rho_\alpha - \sum_{\alpha\beta=1}^{q} u_{\alpha\beta}\rho_\alpha\rho_\beta \ , \qquad \rho_\alpha = a_i^\dagger a_j \ , \qquad \rho_\beta = a_k^\dagger a_l \end{aligned} \tag{4}$$

can be brought into the form (3) by diagonalizing $u_{\alpha\beta}$, with the number q of separable interactions V_α^2 equals at most to the square of the number of single particle states. In order to obtain a path integral representation of $U = \exp(-\beta H)$ we divide the imaginary-time interval $[0, \beta)$ into N sub-intervals of length $\epsilon = \beta/N$ and write

$$U = \prod_{n=1}^{N} e^{-K\epsilon + \frac{1}{2}\chi V^2 \epsilon} = \left[\prod_{n=1}^{N} e^{-K\epsilon} e^{\frac{1}{2}\chi V^2 \epsilon} \times \left(1 + \mathcal{O}(\epsilon^2)\right)\right] \ , \tag{5}$$

At each time slice n we use the identity

$$e^{\lambda \hat{a}^2} = \sqrt{\frac{\lambda}{\pi}} \int_{-\infty}^{\infty} d\xi e^{-\lambda\xi^2} e^{\pm 2\lambda\xi\hat{a}} \ , \tag{6}$$

valid for any operator $\hat{a}$ with a bounded spectrum and $\lambda > 0$ (we shall comment on the case $\lambda < 0$ below), to replace $e^{\frac{1}{2}\chi V^2 \epsilon}$ by an integral over an auxiliary variable ξ_n. This is the Hubbard-Stratonovich (HS) transformation [6], resulting in

$$U = \left(\frac{\chi\epsilon}{2\pi}\right)^{\frac{N}{2}} \int \prod_{n=1}^{N} d\xi_n \exp\left(-\frac{1}{2}\chi\epsilon \sum_{n=1}^{N} \xi_n^2\right) \prod_{n=1}^{N} e^{-K\epsilon + \chi\xi_n V\epsilon} \ . \tag{7}$$

In the limit $N \to \infty$, ξ_n becomes a field $\xi(\tau = n\epsilon) = \xi_n$ and we obtain the continuous version of the HS transformation

$$U = \int \mathcal{D}[\xi] \exp\left[-\frac{1}{2}\chi \int_0^\beta d\tau \xi^2(\tau)\right] U_\xi \ , \tag{8}$$

where U_ξ is the (imaginary time) propagator for a time-dependent one-body Hamiltonian $H_\xi = K - \chi\xi(\tau)V$

$$U_\xi = \mathrm{T}\exp\left\{-\int_0^\beta d\tau\left[K - \chi\xi\left(\tau\right)V\right]\right\} , \tag{9}$$

and T denote time ordering. Eq.(8) provides a representation of the many-body evolution operator as an average over one-body evolutions U_ξ which correspond to non-interacting particles moving in a fluctuating time-dependent field $\xi(\tau)$, weighted by a Gaussian factor. Following [22] it is advantageous to describe the field $\xi(\tau)$ in terms of its Fourier components,

$$\xi(\tau = n\epsilon) = \sum_{r=-(N-1)/2}^{(N-1)/2} \sigma_r e^{i\omega_r\tau} , \tag{10}$$

where $\sigma_{-r} = \sigma_r^*$ to keep $\xi(\tau)$ real and $\omega_r = 2\pi r/\beta$ are the Matsubara frequencies. Here we assume the number of time slices N to be odd. Rewriting the functional integral over the field in terms of σ_r, we have

$$U = \int \mathcal{D}[\sigma]\exp\left(-\frac{1}{2}\chi\beta\sum_r \mid \sigma_r \mid^2\right)U_\sigma , \tag{11}$$

where

$$U_\sigma = \mathrm{T}\exp\left[-\int_0^\beta d\tau\left(K - \chi\sigma_0 V - \chi\sum_{r\neq 0}\sigma_r e^{i\omega_r\tau}V\right)\right] . \tag{12}$$

The measure in (11) is given by

$$\mathcal{D}[\sigma] = (\chi\beta)^{\frac{N}{2}}\frac{d\sigma_0}{\sqrt{2\pi}}\prod_{r>0}\frac{d\sigma_r' d\sigma_r''}{\pi} , \tag{13}$$

where $\sigma_r = \sigma_r' + i\sigma_r''$. The one-body Hamiltonian H_σ whose corresponding propagator is U_σ separates into static and time-dependent parts

$$\begin{aligned} H_\sigma &= h_0 + h_1 , \\ h_0 &= K - \chi\sigma_0 V , \qquad h_1 = -\chi\sum_{r\neq 0}\sigma_r e^{i\omega_r\tau}V . \end{aligned} \tag{14}$$

It is useful to introduce the interaction picture representation $\mathcal{U}_\sigma$ of the one-body propagator U_σ with respect to the static part of the Hamiltonian h_0

$$U_\sigma = e^{-\beta h_0}\mathrm{T}\exp\left[\int_0^\beta d\tau h_1\left(\tau\right)\right] \equiv e^{-\beta h_0}\mathcal{U}_\sigma , \tag{15}$$

where $h_1(\tau) = e^{\tau h_0}h_1 e^{-\tau h_0}$. We then rewrite (11) as

$$U = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} e^{-\beta h_0} \times \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} \mid \sigma_r \mid^2\right) \mathcal{U}_\sigma \tag{16}$$

with the measure

$$\mathcal{D}'[\sigma] = (\chi\beta)^{\frac{N-1}{2}} \prod_{r>0} \frac{d\sigma_r' d\sigma_r''}{\pi} . \tag{17}$$

Eq. (16) describes the evolution operator for the two-body H as a Gaussian-weighted average of one-body evolutions $e^{-\beta h_0}$ corresponding to a static field σ_0, multiplied by a correction factor which represents the contribution from time-dependent fluctuations of the ξ-field about σ_0. In fact, as we demonstrate below, any quantity of interest can be written as an integral over its static-field value times a correction factor. The objective of this paper is to approximate this factor for various quantities by evaluating the small-amplitude fluctuation contribution to the integral over $\sigma_r (r > 0)$ and to explore the validity of this approximation.

For a superposition of separable interactions (3) one introduces auxiliary-field variables σ_r^α corresponding to each V_α but the preceding development remains unchanged. We point out that for $\chi < 0$ in (1) one should use

$$e^{-\lambda\hat{a}^2} = \sqrt{\frac{\lambda}{\pi}} \int_{-\infty}^{\infty} d\xi e^{-\lambda\xi^2} e^{\pm 2i\lambda\xi\hat{a}} \tag{18}$$

($\lambda > 0$) instead of (6).

III. PARTITION FUNCTION

We now consider the partition function $Z \equiv \mathrm{Tr} e^{-\beta H}$. We work in the grand canonical ensemble and set the chemical potential $\mu = 0$ to keep the notation simple. It is convenient to choose a σ_0-dependent basis for the Fock space in which h_0 is diagonal:

$$h_0 = \sum_i \epsilon_i(\sigma_0) a_i(\sigma_0)^\dagger a_i(\sigma_0) , \qquad V = \sum_{ij} v_{ij}(\sigma_0) a_i(\sigma_0)^\dagger a_j(\sigma_0) . \tag{19}$$

We can write Z using (11) as

$$Z = \mathrm{Tr} U = \int \mathcal{D}[\sigma] \exp\left(-\frac{1}{2}\chi\beta \sum_r \mid \sigma_r \mid^2\right) \mathrm{Tr} U_\sigma \equiv \int \mathcal{D}[\sigma] e^{-\beta F(\beta;\sigma)} , \tag{20}$$

or in a form more convenient for our purpose (using (16)):

$$Z = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} \zeta_0 \zeta_0' \equiv \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\beta F_0(\beta;\sigma_0)} . \tag{21}$$

Here

$$\zeta_0 = \mathrm{Tr} e^{-\beta h_0} = \prod_i \left[1 + e^{-\beta\epsilon_i(\sigma_0)}\right] \tag{22}$$

is the partition function corresponding to the static part h_0 and

$$\zeta_0' = \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} \mid \sigma_r \mid^2\right) \frac{1}{\zeta_0} \mathrm{Tr}\left(e^{-\beta h_0} \mathcal{U}_\sigma\right) = \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} \mid \sigma_r \mid^2\right) \langle \mathcal{U}_\sigma \rangle_0 \quad (23)$$

is the correction factor to ζ_0 due to the time-dependent fluctuations of the field about σ_0. We use the notation $\langle O \rangle_0 \equiv \mathrm{Tr}(e^{-\beta h_0} O)/\zeta_0$ to denote the thermal average of an observable O with respect to h_0. The effective static-field free energy F_0 is defined by (21) to be

$$F_0(\beta; \sigma_0) = \frac{1}{2}\chi\sigma_0^2 - \frac{1}{\beta}\log\zeta_0 - \frac{1}{\beta}\log\zeta_0' \; . \tag{24}$$

The representation (21) of Z is a starting point for various approximations. The mean-field approximation (MFA) is obtained when the contribution of the time-dependent paths to Z is neglected by setting $h_1 = 0$, implying $\zeta_0' = 1$, and the integration over the static fields σ_0 is performed in the method of steepest descent. This amounts to approximating the path integral by the contributions of the static paths $\bar{\sigma}_0$ that minimize the free energy F_0 in (24). It is easy to show [2,5] that this minimization condition is

$$\bar{\sigma}_0 = \langle V \rangle_0 = \sum_i v_{ii}(\bar{\sigma}_0) f_i(\bar{\sigma}_0) \; , \tag{25}$$

where $f_i = (1 + e^{\beta\epsilon_i})^{-1}$ are the Fermi occupation numbers, and that the solution $\bar{\sigma}_0$ of (25) is the Hartree mean field. One can improve on the MFA result by performing the integration over σ_r in the expression (23) for ζ_0' also by steepest descent. The saddle point is now given by $\bar{\sigma}_0, \sigma_r = 0$ and one obtains the finite temperature RPA corrections to the partition function [5].

The static-path approximation (SPA) [11] – [17] is obtained by again setting $h_1 = 0$ but now the integration over σ_0 in (21) is performed exactly, thus approximating the path integral by the contributions from all static paths:

$$Z^{(SPA)} = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} \zeta_0 = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} \prod_i \left[1 + e^{-\beta\epsilon_i(\sigma_0)}\right] \; . \tag{26}$$

The SPA is expected to become exact at high temperatures since one can use the one time slice approximation in (7) with an error of $\mathcal{O}(\beta^2)$ that vanishes as $T \to \infty$. This method is advantageous to the MFA since it takes into account exactly large amplitude static fluctuations around the mean field. However, it neglects the time-dependent fluctuations which constitute the RPA corrections. This shortcoming of the SPA can be remedied if the exact integration over the static paths is supplemented by evaluation of ζ_0' in the limit of small amplitude time-dependent fluctuations about each static value σ_0. This scheme, the perturbed static-path approximation (PSPA), is the focus of our work. It was introduced in Refs. [18] - [21] for the partition function Z. Our approach is different and has the advantage that it can be generalized to the calculation of observables and response functions as shown in the following sections. We first illustrate our method by rederiving the corresponding expression for the partition function. We expand $\log\langle \mathcal{U}_\sigma \rangle_0$ in (23)

$$\log\langle\mathcal{U}_\sigma\rangle_0 = \chi\sum_{r\neq 0}\sigma_r\int_0^\beta d\tau e^{i\omega_r\tau}\langle V(\tau)\rangle_c$$
$$+\frac{1}{2}\chi^2\sum_{rs\neq 0}\sigma_r\sigma_s\int_0^\beta d\tau d\tau' e^{i\omega_r\tau}e^{i\omega_s\tau'}\left[\langle \mathrm{T}V(\tau)V(\tau')\rangle_c - \langle V(\tau)\rangle_c\langle V(\tau')\rangle_c\right]$$
$$+\mathcal{O}\left(\sigma^3\right)\ , \tag{27}$$

with $V(\tau) = e^{\tau h_0}Ve^{-\tau h_0}$ in the interaction picture. The time-ordered averages are calculated using the finite-temperature Wick's theorem [1,2] where the subscript c means that only the connected diagrams should be summed up in the diagrammatic representation of this expansion.

The first term in (27) vanishes since $\langle V(\tau)\rangle_c$ is τ-independent. For the second term Wick's theorem gives

$$\langle \mathrm{T}V(\tau)V(\tau')\rangle_c = -\sum_{ij} v_{ij}v_{ji}g_i^0(\tau'-\tau)g_j^0(\tau-\tau')\ , \tag{28}$$

where the unperturbed temperature Green's function g_i^0 is given by

$$g_i^0(\tau-\tau') = -\langle a_i(\tau)a_i^\dagger(\tau')\rangle_0 = \frac{1}{\beta}\sum_{k=-\infty}^{\infty}\frac{e^{-i\nu_k(\tau-\tau')}}{i\nu_k-\epsilon_i} \tag{29}$$

with frequencies $\nu_k = (2\pi+1)k/\beta$. Using (28-29) we obtain for the double integral in (27)

$$\int_0^\beta d\tau d\tau'\cdots = -\delta_{r,-s}\sum_{ij}v_{ij}v_{ji}\sum_{k=-\infty}^{\infty}\frac{1}{i\nu_k-\epsilon_i}\,\frac{1}{i\nu_k-(\epsilon_j-i\omega_r)}\ . \tag{30}$$

The infinite sum over k in (30) is calculated using the frequency summation technique [1,2]. The essence of this method lies in the observation that the points $z = i\nu_k$ are the poles of the function $-\beta/(e^{\beta z}+1)$ with residue of one and the sum therefore equals the contour integral

$$\sum_{k=-\infty}^{\infty}\frac{1}{i\nu_k-\epsilon_i}\,\frac{1}{i\nu_k-(\epsilon_j-i\omega_r)} = \frac{1}{2\pi i}\oint_{\mathcal{C}} dz\,\frac{-\beta}{e^{\beta z}+1}\,\frac{1}{z-\epsilon_i}\,\frac{1}{z-(\epsilon_j-i\omega_r)}\ , \tag{31}$$

where $\mathcal{C}$ encircles the imaginary axis. This contour can be continuously transformed into a circle centered at the origin of an arbitrarily large radius, which is deformed at two places to include the poles at $z=\epsilon_i$ and $z=\epsilon_j-i\omega_r$. The residue theorem then gives

$$\int_0^\beta d\tau d\tau'\cdots = -\beta\delta_{r,-s}\sum_{ij}v_{ij}v_{ji}\frac{f_i-f_j}{\Delta_{ij}+i\omega_r}\ , \tag{32}$$

with $\Delta_{ij}=\epsilon_i-\epsilon_j$. Using (32) in (27) we have

$$\langle\mathcal{U}_\sigma\rangle_0 = \exp\left(-\chi\beta\sum_{r>0}a_r\mid\sigma_r\mid^2\right)\ , \tag{33}$$

with

$$a_r(\sigma_0) = \chi \sum_{ij} v_{ij} v_{ji} \frac{f_i - f_j}{\Delta_{ij} + i\omega_r} = \chi \sum_{ij} v_{ij} v_{ji} \frac{(f_i - f_j)\,\Delta_{ij}}{\Delta_{ij}^2 + \omega_r^2} \ . \tag{34}$$

The correction factor ζ_0' in (23) is now given by a Gaussian integral and we obtain

$$\zeta_0' = \prod_{r>0} (1 + a_r)^{-1} = \prod_{r>0} \frac{\prod'_{ij} \left(\omega_r^2 + \Delta_{ij}^2\right)}{\prod_\nu (\omega_r^2 + \Omega_\nu^2)} = \frac{\prod'_{ij} \frac{1}{\Delta_{ij}} \sinh \frac{\beta \Delta_{ij}}{2}}{\prod_\nu \frac{1}{\Omega_\nu} \sinh \frac{\beta\Omega_\nu}{2}} \ . \tag{35}$$

The second equality in (35) defines the frequencies $\Omega_\nu(\beta, \sigma_0)$ through [20]

$$1 + a_r = \frac{\prod'_{ij}(\omega_r^2 + \Delta_{ij}^2) + 2\chi \sum'_{ij} v_{ij} v_{ji} (f_i - f_j) \Delta_{ij} \prod'_{kl \neq ij} (\omega_r^2 + \Delta_{kl}^2)}{\prod'_{ij}(\omega_r^2 + \Delta_{ij}^2)} \equiv \frac{\prod_\nu (\omega_r^2 + \Omega_\nu^2)}{\prod'_{ij}(\omega_r^2 + \Delta_{ij}^2)} \ , \tag{36}$$

where the prime in $\prod'_{ij}$ and $\sum'_{ij}$ restricts the product or sum to pairs (i,j) that satisfy $i < j$ and $\Delta_{ij} \neq 0$. Note that there are as many Ω_ν in the numerator of (36) as there are Δ_{ij} in the denominator. The third equality in (35) uses the infinite product representation $\sinh x = x \prod_{r>0} (1 + x^2/\pi^2 r^2)$. Together with (21) and (22) we finally have

$$Z^{(PSPA)} = \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} \prod_i \left(1 + e^{-\beta\epsilon_i(\sigma_0)}\right) \frac{\prod'_{ij} \frac{1}{\Delta_{ij}} \sinh \frac{\beta\Delta_{ij}}{2}}{\prod_\nu \frac{1}{\Omega_\nu} \sinh \frac{\beta\Omega_\nu}{2}} \ . \tag{37}$$

This is a closed-form expression which corresponds to the limit $N \to \infty$ (N is the number of imaginary-time slices, see (5)) since the infinite product in (35) has been performed exactly. Hence the PSPA result does not contain errors originating from a discretization of $[0, \beta)$ into sub-intervals of a finite length, as is the case in a Monte Carlo evaluation of the path integral.

$\omega = \pm\Omega_\nu$ are the roots of $1 + \sum_{ij} v_{ij} v_{ji} (f_i - f_j)/(\Delta_{ij} + i\omega) = 0$. It can be shown [20] that for the value $\sigma_0 = \bar{\sigma}_0(\beta)$ which minimizes $F_0(\beta; \sigma_0)$ (see Eqs. (24) and (25)), these roots $\pm\Omega_\nu$ are the RPA frequencies, i.e. the frequencies of small amplitude oscillations around the equilibrium configuration. For an arbitrary static σ_0, the frequencies $\omega = \pm\Omega_\nu$ solve the generalized finite temperature RPA equations obtained by replacing the equilibrium configuration by the arbitrary σ_0 (see Appendix A). We note that the Gaussian approximation in (23) leads to a convergent integral only if $1 + a_r > 0$ for all r, i.e. $-\Omega_\nu^2 < \omega_r^2$ for all r and ν. When all RPA frequencies are real, these conditions are always met. In particular this is the case if σ_0 is a local minimum of the static free energy i.e. a stable mean-field configuration $\bar{\sigma}_0$ (Thouless theorem [23]). At zero temperature $\omega_r = 0$ and an imaginary RPA frequency would lead to a breakdown of the Gaussian approximation. However, at finite temperature imaginary RPA frequencies do not necessarily lead to instability. If the largest modulus of all imaginary RPA frequencies is below $\omega_1 = 2\pi T$, then the quadratic fluctuations in σ_r are still stable. An instability in the σ_1 direction occurs when the magnitude of one of

the imaginary RPA frequencies crosses $2\pi T$. The RPA frequencies depend both on β and σ_0. In particular, for any temperature β^{-1} there exists a static field $\sigma_0 = \sigma_0'(\beta)$ such that $\Omega_\nu^2(\beta, \sigma_0') = -\omega_1^2 = -(2\pi/\beta)^2$ for some ν, causing the correction factor ζ_0' to diverge. Note that at $T = 0$ instability occurs as soon as some Ω_ν becomes imaginary whereas at $T > 0$ an instability develops only for a sufficiently imaginary Ω_ν. These instabilities can be ignored when they occur at fields for which the static free energy is large. In practical applications the PSPA breaks down only at temperatures that are significantly below the shape transition temperature, when the saddle point in the static free energy surface becomes unstable to small amplitude time-dependent fluctuations.

In the case (3) where the interaction is a sum of several separable interactions we have an auxiliary-field variable σ_r^α for each V_α. Assuming $\chi_\alpha = \chi$ (this is always possible by redefining V_α), expression (33) becomes

$$\langle \mathcal{U}_\sigma \rangle_0 = \exp\left(-\chi\beta \sum_r \sum_{\alpha\gamma} \sigma_r^{\alpha *} a_r^{\alpha\gamma} \sigma_r^\gamma \right) \tag{38}$$

with

$$a_r^{\alpha\gamma}(\sigma_0) = \chi \sum_{ij} v_{ij}^\alpha v_{ji}^\gamma \frac{(f_i - f_j)}{\Delta_{ij} + i\omega_r} \ . \tag{39}$$

The correction factor ζ_0' is then generalized from (35) into

$$\zeta_0' = \prod_{r>0} \det\left(1 + a_r\right)^{-1} \tag{40}$$

where a_r is the q-dimensional matrix defined in (39). As shown in Appendix A

$$\det(1 + a_r) = \frac{\prod_\nu (\omega_r^2 + \Omega_\nu^2)}{\prod_{ij}{}'(\omega_r^2 + \Delta_{ij}^2)} \ , \tag{41}$$

where Ω_ν are again the RPA frequencies at finite temperature. We then obtain for the PSPA partition function an expression similar to (37), except that the integral over σ_0 is replaced by an integration over q static fields σ_0^α.

When one or more of the χ_α in (3) are negative and a representation of the type (18) is used in the HS transformation, the one-body Hamiltonian h_0 in (19) becomes non-hermitean, so that its eigenvalues $\epsilon_i(\sigma_0)$ are in general complex and the associated one-body partition function can be negative. It was recently pointed out [24] that the static fields which correspond to these "repulsive" terms in the interaction do not represent large amplitude thermal fluctuations, and can simply be treated in a saddle point approximation. This amounts to keeping the exact integration over the static "attractive" fields but taking the mean-field solution for the static "repulsive" fields for every configuration of the "attractive" fields in the integrand.

An alternative way to approach "repulsive" interactions is to subtract from the Hamiltonian a term proportional to $\hat{N}^2$ ($\hat{N}$ is the particle number operator) with a coefficient large enough so that the two-body part of the Hamiltonian becomes a negative-definite quadratic

form (as in the case where all χ_α in (3) are positive). However, by doing this we also increase the magnitude of "attractive" terms and it remains to be investigated whether the SPA and PSPA would still work well for such modified Hamiltonians. Note that the subtracted term is just a constant for a fixed number of particles.

To illustrate our results we apply the formalism to a simple many-body model (a variant of the Lipkin model [25]) based on a $U(2)$ algebra which is defined and solved in Appendix B. At each σ_0 we have

$$h_0 = 2\epsilon J_z - 2\chi\sigma_0 J_x \ , \qquad h_1 = -2\chi \sum_{r\neq 0} \sigma_r e^{i\omega_r \tau} J_x \ . \tag{42}$$

Thus the single-particle Hamiltonian corresponding to h_0 has two g-fold degenerate levels $\epsilon_i = \pm\bar{\epsilon}$ where $\bar{\epsilon} = \sqrt{\epsilon^2 + \chi^2\sigma_0^2}$, so $\Delta_{ij} = 0, \pm 2\bar{\epsilon}$. The matrix corresponding to $V = 2J_x$ is block-diagonal with g 2×2-blocks

$$v_{ij} = \begin{pmatrix} -\sin 2\phi & \cos 2\phi \\ \cos 2\phi & \sin 2\phi \end{pmatrix} \ , \qquad \sin 2\phi = \frac{\chi\sigma_0}{\bar{\epsilon}} \ , \qquad \cos 2\phi = \frac{\epsilon}{\bar{\epsilon}} \tag{43}$$

and the matrix

$$p_{ij} = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \tag{44}$$

diagonalizes the 2×2-blocks of h_0. For ζ_0 and ζ_0' we obtain

$$\zeta_0 = \left(2\cosh\frac{\beta\bar{\epsilon}}{2}\right)^{2g} \ , \qquad \zeta_0' = \frac{\Omega}{2\bar{\epsilon}} \frac{\sinh\beta\bar{\epsilon}}{\sinh\frac{\beta\Omega}{2}} \ , \tag{45}$$

where $\Omega^2 = 4\bar{\epsilon}^2 - (4g\epsilon^2\chi/\bar{\epsilon})\tanh(\beta\bar{\epsilon}/2)$, so there are only two RPA frequencies $\pm\Omega$. The saddle-point mean-field equation (25) is

$$\tanh\frac{\beta\bar{\epsilon}}{2} = \frac{\bar{\epsilon}}{g\chi} \tag{46}$$

and has a single spherical stable solution $\sigma_0 = 0$ for $\beta < \beta_c$, which becomes unstable for $\beta > \beta_c$ and bifurcates into two deformed minima $\sigma_0 = \pm\bar{\sigma}_0(\beta)$. Here β_c is the transition temperature

$$\beta_c = \frac{1}{\epsilon}\log\frac{\kappa+1}{\kappa-1} \ , \qquad \kappa = \frac{g\chi}{\epsilon} \ . \tag{47}$$

The dimensionless parameter κ thus determines the mean-field behavior of the model. For $\kappa < 1$ there is no phase transition and $\sigma_0 = 0$ is the only solution at all temperatures.

In Fig. 1 we present the MFA, SPA and PSPA results for the free energy $F(\beta) \equiv -\beta^{-1}\log Z$ in our $U(2)$ model using $\epsilon = 1$ and $g = 10$ and compare them against the exact result. We consider three cases characterized by different values of κ. For $\kappa = 0.5$ there is no mean-field transition whereas for $\kappa = 1.5$ and $\kappa = 3.0$ the signature of a transition at temperatures $\beta_c = 1.61$ and $\beta_c = 0.693$, respectively, is seen in the mean-field curve. The

SPA overestimates the exact result especially at low T whereas the PSPA is quite accurate at all temperatures. All three approximations converge to the exact result as $T \to \infty$. We find that for β sufficiently small the divergence of ζ_0' occurs only at a very large $\sigma_0 = \sigma_0'(\beta)$, where the other factors in the integrand of (37) are vanishingly small, and therefore does not constitute a practical problem. The breakdown of the PSPA occurs when β becomes large enough such that $\sigma_0'(\beta) \sim 0$. This happens only at temperatures far below the transition temperature $T_c = 1/\beta_c$.

In order to study the effect of the time-dependent fluctuations we compare in Fig. 2 the effective free energy $F_0(\beta; \sigma_0)$ in (24) as a function of the static field σ_0 with the SPA free energy ($\zeta_0' = 1$ in (24)) at different temperatures. We consider the case $\kappa = 1.5$. Above the mean-field transition temperature $\beta_c = 1.61$, $\zeta_0' \approx 1$ and the two approximations yield similar results. As the temperature is lowered, time-dependent fluctuations deepen the free-energy minimum at $\sigma_0 = 0$. Below T_c these fluctuations also lower the barrier between the two mean-field configurations $\sigma_0 = \pm\bar{\sigma}_0$. Thus the PSPA result for the free energy improves significantly the SPA result especially below the transition temperature (see the middle panel of Fig. 1). The MFA result for the free energy $F(\beta)$ is the most inaccurate especially near the transition where the free energy has comparable values over a broad range of configurations σ_0.

We remark that in spite of its simplicity, the $U(2)$ model has features that are generic to more realistic nuclear interactions (e.g. quadrupole interaction). In particular, the phase transition in its mean-field theory is analogous to the shape transitions from deformed to spherical shapes that occur in deformed nuclei [26]. We therefore expect the PSPA to improve significantly on the SPA also for more realistic nuclear shell model interactions. For interactions that include both pairing and multipole components (e.g. pairing plus quadrupole model), the SPA works better when a mixed pairing-density decomposition is used rather than just a pure density decomposition [9]. A mixed decomposition is thus preferable when the PSPA is applied to such interactions.

IV. THERMAL EXPECTATION VALUES OF OBSERVABLES

In this Section we consider an observable O and treat its expectation value at finite temperature $\langle O \rangle = \mathrm{Tr}(e^{-\beta H} O)/\mathrm{Tr}(e^{-\beta H})$ in the framework of the PSPA. Although we discuss observables of the form $O = D$ and $O = D^2$ for a one-body operator D, any n-body O can be treated in a similar fashion.

A. One-Body Observables

In constructing an auxiliary-field path integral representation for $\langle D \rangle$ we can use Eqs. (11) and (20) to get

$$\langle D \rangle = \frac{\int \mathcal{D}[\sigma] e^{-\beta F(\beta;\sigma)} \langle D \rangle_\sigma}{\int \mathcal{D}\sigma e^{-\beta F_\sigma}} \,, \qquad \langle D \rangle_\sigma = \frac{\mathrm{Tr}(U_\sigma D)}{\mathrm{Tr} U_\sigma} \,. \tag{48}$$

Alternatively, to facilitate our calculations we can use (16) and (21) to write

$$\langle D \rangle = \frac{\int d\sigma_0 e^{-\beta F_0} D_0}{\int d\sigma_0 e^{-\beta F_0}} \tag{49}$$

where

$$D_0 = \frac{1}{\zeta_0'} \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} \mid \sigma_r \mid^2\right) \langle \mathcal{U}_\sigma D \rangle_0 \ . \tag{50}$$

The effective static-field free energy $F_0(\beta;\sigma_0)$, defined in (24), has been calculated in the previous Section (see Eqs. (22) and (35)). Our aim here is to calculate D_0. In a diagrammatic representation of the perturbation series for $\langle \mathcal{U}_\sigma D \rangle_0$ the connected diagrams can be easily shown to factor out at each order [1,2]:

$$\langle \mathcal{U}_\sigma D \rangle_0 = \langle \mathcal{U}_\sigma \rangle_0 \langle \mathcal{U} \sigma D \rangle_c \ . \tag{51}$$

Thus we can write D_0 itself as a weighted average of $\langle \mathcal{U}_\sigma D \rangle_c$:

$$D_0 = \frac{\int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} \mid \sigma_r \mid^2\right) \langle \mathcal{U}_\sigma \rangle_0 \langle \mathcal{U}_\sigma D \rangle_c}{\int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} \mid \sigma_r \mid^2\right) \langle \mathcal{U}_\sigma \rangle_0} \ . \tag{52}$$

$\langle \mathcal{U}_\sigma \rangle_0$ is given in (33) and (34), whereas for $\langle \mathcal{U}_\sigma D \rangle_c$ we expand

$$\langle \mathcal{U}_\sigma D \rangle_c = \langle D \rangle_0 + \frac{1}{2}\chi^2 \sum_{rs \neq 0} \sigma_r \sigma_s \int_0^\beta d\tau d\tau' e^{i\omega_r \tau} e^{i\omega_s \tau'} \langle \mathrm{T} V(\tau) V(\tau') D(0) \rangle_c + \mathcal{O}(\sigma^3) \ . \tag{53}$$

Notice the absence of first-order terms in σ_r since they vanish upon the integration in (52).

Before continuing we introduce the following notation. Using (23) and (33) we define a matrix $A(\sigma_0)$ by

$$\zeta_0' = \int \mathcal{D}'[\sigma] \exp\left[-\chi\beta \sum_{r>0} (1 + a_r) \mid \sigma_r \mid^2\right] \equiv \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sigma^T A \sigma\right) \ , \tag{54}$$

where the vector σ has $N-1$ components $(\sigma_1', \sigma_2', \cdots, \sigma_1'', \sigma_2'', \cdots)$ and A is diagonal with elements $(1 + a_1, 1 + a_2, \cdots, 1 + a_1, 1 + a_2, \cdots)$ with a_r given in (34). We also use (53) to define $b(\sigma_0)$ and a matrix $B(\sigma_0)$ by

$$\langle \mathcal{U} D \rangle_c \equiv b + \frac{1}{2} \sigma^T B \sigma \ . \tag{55}$$

Using this notation we find

$$\begin{aligned} D_0^{(SPA)} &= b(\sigma_0) \ , \\ D_0^{(PSPA)} &= b(\sigma_0) + \frac{1}{4\chi\beta} \mathrm{Tr}\left[A^{-1}(\sigma_0) B(\sigma_0)\right] \ . \end{aligned} \tag{56}$$

Recall that at each σ_0 we choose a different basis (19) for the Fock space in which we write

$$D = \sum_{ij} d_{ij}(\sigma_0) a_i(\sigma_0)^\dagger a_j(\sigma_0) \ . \tag{57}$$

The zeroth-order term is then

$$b(\sigma_0) = \langle D \rangle_0 = \sum_i d_{ii} f_i \ . \tag{58}$$

In order to obtain an expression for $\mathrm{Tr}(A^{-1}B)$ in (56) we calculate the double integral in (53) using Wick's theorem and the frequency summation technique [1,2]. Notice that since A is diagonal it is sufficient to consider the case $s = -r$. The calculation is similar to the one performed in the previous Section and yields the result

$$\mathrm{Tr}(A^{-1}B) = 2\chi^2 \sum_{ijk} v_{ij} v_{jk} d_{ki} \sum_{r \neq 0} a_r^{-1} I_r^{ijk} \ , \tag{59}$$

where

$$I_r^{ijk} = \frac{f_i}{(\Delta_{ij} - i\omega_r)\Delta_{ik}} - \frac{f_j}{(\Delta_{ij} - i\omega_r)(\Delta_{jk} + i\omega_r)} + \frac{f_k}{\Delta_{ik}(\Delta_{jk} + i\omega_r)} \ . \tag{60}$$

In the cases $\epsilon_j = \epsilon_i$ etc. it is understood that $I_r^{ijk} \equiv \lim\limits_{\epsilon_j \to \epsilon_i} I_r^{ijk}$.

The sum over $r \neq 0$ in (59) which consists of $N-1$ elements can be expressed in a closed form for $N \to \infty$ by applying once more the frequency summation technique. Writing $a_r^{-1} = a^{-1}(i\omega_r)$ and $I_r^{ijk} = I^{ijk}(i\omega_r)$, we observe that the sum is carried out over the points $z = i\omega_r$ which are the poles of the function $\beta/(e^{\beta z} - 1)$ with residue of one. Therefore

$$\sum_{r \neq 0} a_r^{-1}(i\omega_r) I_r^{ijk}(i\omega_r) = \frac{1}{2\pi i} \oint_{\mathcal{C}} dz \frac{\beta}{e^{\beta z} - 1} a^{-1}(z) I^{ijk}(z) \ - \ a^{-1}(0) I^{ijk}(0) \ , \tag{61}$$

where the contour $\mathcal{C}$ encircles the imaginary axis. To evaluate the integral we transform $\mathcal{C}$ into an arbitrarily large circle, deformed to include the poles at $z = \Delta_{ij}$, $z = -\Delta_{jk}$, and $z = \pm\Omega_\nu$ for all ν, and obtain

$$\begin{aligned} D_0^{(SPA)} &= \sum_i d_{ii} f_i \ , \\ D_0^{(PSPA)} &= \sum_i d_{ii} f_i - \frac{\chi}{2\beta} \sum_{ijk} v_{ij} v_{jk} d_{ki} \left[\sum_\alpha \frac{\beta}{e^{\beta z_\alpha} - 1} \frac{p_{ijk}(z_\alpha)}{\prod\limits_{\alpha' \neq \alpha} (z_\alpha - z_{\alpha'})} + \frac{p_{ijk}(0)}{\prod\limits_{\alpha'} (-z_{\alpha'})} \right] \ . \end{aligned} \tag{62}$$

Here

$$\begin{aligned} p_{ijk}(z) &= \left[\frac{f_k}{\Delta_{ik}} (z - \Delta_{ij}) - \frac{f_i}{\Delta_{ik}} (z + \Delta_{jk}) + f_j \right] \prod_{lm}{}' (z^2 - \Delta_{lm}^2) \ , \\ z_\alpha &= \Delta_{ij}, -\Delta_{jk}, \pm\Omega_\nu \end{aligned} \tag{63}$$

and the prime in $\prod_{lm}{}'$ restricts the product to pairs (l, m) satisfying $l < m$ and $\Delta_{lm} \neq 0$.

In the case of $q > 1$ separable interactions in (3) the calculation is more complicated since the matrix $A(\sigma_0)$ in (56) is block-diagonal with blocks of dimension $2q$ (see Eqs. (38)-(40)). However, the general form (59) including the summation over r still holds and the subsequent use of frequency summations to get a closed-form result can be carried out in this case as well.

We test the approximations (62) by applying them to the calculation of $\langle J_z \rangle$ in our $U(2)$ model ($\langle J_x \rangle = \langle J_y \rangle = 0$ both exactly and in the above approximations). The matrix corresponding to $D = J_z$ is block-diagonal with g 2×2-blocks

$$d_{ij} = \frac{1}{2} \begin{pmatrix} \cos 2\phi & \sin 2\phi \\ \sin 2\phi & -\cos 2\phi \end{pmatrix} \tag{64}$$

in the notation of (43)-(44). Thus

$$\langle J_z \rangle^{(SPA)} = \frac{1}{Z^{(SPA)}} \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} \left(2\cosh\frac{\beta\bar{\epsilon}}{2} \right)^{2g} \times \frac{-g}{2} \cos 2\phi \tanh\frac{\beta\bar{\epsilon}}{2} \,. \tag{65}$$

The more complicated expression for $\langle J_z \rangle^{(PSPA)}$ is similarly obtained using (43)-(45) and (62)-(64). The SPA and PSPA results are presented in Fig. 3 together with the mean-field calculation derived from a steepest-descent evaluation of (65). Above the transition temperature all approximations agree fairly well with the exact result (B8). For lower temperatures the MFA and SPA significantly overestimate the exact result whereas the PSPA works well down to the breakdown temperature.

B. Two-Body Observables

For simplicity we assume a two-body observable of the form $O = D^\dagger D$ where D is a one-body operator. The calculation of the expectation value of such an observable, albeit more complicated, can be carried out along the same lines. As for $\langle D \rangle$ we have

$$\langle O \rangle = \frac{\int d\sigma_0 e^{-\beta F_0} O_0}{\int d\sigma_0 e^{-\beta F_0}} \,, \tag{66}$$

where

$$O_0 = \frac{1}{\zeta_0'} \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} |\, \sigma_r \,|^2 \right) \langle \mathcal{U}_\sigma D^\dagger D \rangle_0 \,. \tag{67}$$

Following similar steps we get an expression of the form (56) with the same $A(\sigma_0)$ but different $B(\sigma_0), b(\sigma_0)$. After further manipulations we obtain the final result

$$\begin{aligned} O_0^{(SPA)} &= b(\sigma_0) \,, \\ O_0^{(PSPA)} &= b(\sigma_0) + \frac{\chi}{4\beta} \sum_{u=1}^{6} t_u(\sigma_0) \,, \end{aligned} \tag{68}$$

where

$$
\begin{aligned}
b(\sigma_0) &= \sum_{ij} \left[d^\dagger_{ij} d_{ji} f_i (1 - f_j) + d^\dagger_{ii} d_{jj} f_i f_j \right] \ , \\
t_1(\sigma_0) &= \sum_{ijkl} v_{ij} v_{jk} d_{ki} d^\dagger_{ll} f_l S^{(1)}_{ijk} \ , \\
t_2(\sigma_0) &= \sum_{ijkl} v_{ij} v_{jk} d^\dagger_{ki} d_{ll} f_l S^{(1)}_{ijk} \ , \\
t_3(\sigma_0) &= \sum_{ijkl} v_{ij} v_{kl} d^\dagger_{ji} d_{lk} S^{(2)}_{ijkl} \ , \\
t_4(\sigma_0) &= -\sum_{ijkl} v_{ij} v_{jk} d_{kl} d^\dagger_{li} f_l S^{(1)}_{ijk} \ , \\
t_5(\sigma_0) &= \sum_{ijkl} v_{ij} v_{jk} d^\dagger_{kl} d_{li} (1 - f_l) S^{(1)}_{ijk} \ , \\
t_6(\sigma_0) &= -\sum_{ijkl} v_{ij} v_{kl} d^\dagger_{jk} d_{li} S^{(2)}_{ijkl} \ .
\end{aligned} \tag{69}
$$

$S^{(1)}_{ijk}, S^{(2)}_{ijkl}$ in (69) are given by

$$
\begin{aligned}
S^{(v)} &= -\sum_\alpha \frac{\beta}{e^{\beta z_\alpha} - 1} \frac{q^{(v)}(z_\alpha)}{\prod\limits_{\alpha' \neq \alpha} (z_\alpha - z_{\alpha'})} \ - \ \frac{q^{(v)}(0)}{\prod\limits_{\alpha'} (-z_{\alpha'})} \ , \qquad v = 1, 2 \ , \\
q^{(1)}_{ijk}(z) &= p_{ijk}(z) \quad \text{of (63)} \ , \\
q^{(2)}_{ijkl}(z) &= -(f_i - f_j)(f_k - f_l) \prod_{pq}{}' (z^2 - \Delta^2_{pq}) \ , \\
z_\alpha &= -\Delta_{ij}, \Delta_{jk}, \pm\Omega_\nu \ .
\end{aligned} \tag{70}
$$

To test the approximations (68) we apply them to the calculation of $\langle J_x^2 \rangle$, $\langle J_y^2 \rangle$ and $\langle J_z^2 \rangle$ in our $U(2)$ model. The matrices corresponding to $D = J_z, J_y$ are block-diagonal with g 2×2-blocks

$$
d^{(J_x)}_{ij} = \frac{1}{2} \begin{pmatrix} -\sin 2\phi & \cos 2\phi \\ \cos 2\phi & \sin 2\phi \end{pmatrix} \ , \qquad d^{(J_y)}_{ij} = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{71}
$$

whereas $d^{(J_z)}_{ij}$ is given in (64). We therefore have

$$
\begin{aligned}
\langle D^2 \rangle^{(SPA)} &= \frac{1}{Z^{(SPA)}} \sqrt{\frac{\chi\beta}{2\pi}} \int d\sigma_0 e^{-\frac{1}{2}\chi\beta\sigma_0^2} \left(2\cosh \frac{\beta\bar{\epsilon}}{2} \right)^{2g} \times (D^2)^{(SPA)}_0 \ , \\
(J_x^2)^{(SPA)}_0 &= \frac{g^2}{4} \sin^2 2\phi \tanh^2 \frac{\beta\epsilon}{2} + \frac{g}{8} \left(\cos 4\phi \tanh^2 \frac{\beta\bar{\epsilon}}{2} + 1 \right) \ , \\
(J_y^2)^{(SPA)}_0 &= \frac{g}{8} \left(\tanh^2 \frac{\beta\bar{\epsilon}}{2} + 1 \right) \ , \\
(J_z^2)^{(SPA)}_0 &= \frac{g^2}{4} \cos^2 2\phi \tanh^2 \frac{\beta\epsilon}{2} + \frac{g}{8} \left(-\cos 4\phi \tanh^2 \frac{\beta\bar{\epsilon}}{2} + 1 \right) \ .
\end{aligned} \tag{72}
$$

Expressions for $\langle D^2\rangle^{(PSPA)}$ can similarly be derived using (43)-(45) and (68-71). These results are presented in Fig. 4 together with mean-field calculations for different values of κ. The MFA and SPA exhibit large deviations from the exact results in most cases even above the transition temperature and when no transition occurs. The PSPA shows the best agreement and in the only case where its deviation is appreciable ($\langle J_y^2\rangle$ at $\kappa = 1.5$), the other approximations give qualitatively wrong results. Note that the quantitative differences between the various approximations depend on the observable being calculated. In the no-transition case $\kappa = 0.5$ all approximations agree for $\langle J_z^2\rangle$ (as they do for $\langle J_z\rangle$) but not for $\langle J_x^2\rangle$, $\langle J_y^2\rangle$.

The expectation value of the Hamiltonian $H = 2\epsilon J_z - 2\chi J_x^2$ (B1) itself is shown in Fig. 5 (note that the additivity of the average, $\langle O_1 + O_2\rangle = \langle O_1\rangle + \langle O_2\rangle$, is preserved in MFA, SPA and PSPA). The PSPA result is still superior but the agreement of the SPA with the exact result is also quite good, contrary to what it predicts for $\langle J_z\rangle$ and $\langle J_x^2\rangle$ when taken separately.

V. STRENGTH FUNCTION

A. Linear Response Theory

In this Section we are interested in the response of the system to an external perturbation D as reflected by its thermal strength function

$$G(\omega) = \frac{1}{Z}\sum_{mn} \mid \langle n \mid D \mid m\rangle \mid^2 e^{-\beta E_m}\delta(\omega - E_n + E_m) \ , \tag{73}$$

where $\mid n\rangle$ and E_n are the many-body eigenstates and corresponding energies. $G(\omega)$ is the Fourier transform of the real-time response function $G(t-t')$ which originates in linear-response theory [1,2]

$$G(\omega) = \int\limits_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} G(t) \ ,$$

$$G(t-t') = -i\langle \mathrm{T} D_H^\dagger(t) D_H(t')\rangle = -\frac{i}{Z}\mathrm{Tr}\left[e^{-\beta H}\mathrm{T} D_H^\dagger(t) D_H(t')\right] \ , \tag{74}$$

where the subscript H refers to the Heisenberg picture $D_H(t) = e^{iHt}De^{-iHt}$. If an equilibrated system with a Hamiltonian H is perturbed by some external potential $V(t)$ at $t = t_0$, the change in the thermal expectation value of an observable D with respect to the equilibrium situation is

$$\delta\langle D\rangle(t) = -\frac{i}{\hbar}\int\limits_{t_0}^{t} dt' \langle [D_H(t), V_H(t')]\rangle \Theta(t-t_0) \ . \tag{75}$$

Considering an external perturbation of the form $V(t) = \alpha(t)D = \sum\limits_{ij}\alpha(t)d_{ij}a_i^\dagger a_j$ we can write (75) as

$$\delta\langle D(t)\rangle = \frac{1}{\hbar}\int\limits_{t_0}^{\infty} dt' G^R(t-t')\alpha(t') \ , \tag{76}$$

where

$$G^R(t-t') = -i\langle[D_H(t), D_H(t')]\rangle\Theta(t-t') \tag{77}$$

is the retarded real-time response function. The Fourier transform of the latter is related to that of $\delta\langle D\rangle(t)$ by

$$\delta\langle D\rangle(\omega) = \frac{2\pi}{\hbar}\alpha(\omega)G^R(\omega) \ , \qquad G^R(\omega) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} dt e^{i\omega t} G^R(t) \ . \tag{78}$$

The strength function can also be obtained directly from $G^R(\omega)$:

$$G(\omega) = -\frac{1}{\pi}\frac{1}{1-e^{-\beta\omega}}\mathrm{Im}G^R(\omega) \ . \tag{79}$$

This suggests that in order to approximate $G(\omega)$ we should approximate $G(t)$ or $G^R(t)$ and Fourier-transform the result. This has been done in [16] where $G(\omega)$ has been obtained from a static-path calculation of $G(t)$. However, it is very difficult to incorporate the contribution of time-dependent paths into the real-time formalism. In contrast, the imaginary-time framework discussed in the previous Sections is quite suitable for this task. Thus instead of $G(t)$ we consider the imaginary-time response function [1,2]

$$\mathcal{G}(\tau-\tau') = -\langle \mathrm{T} D_H^\dagger(\tau) D_H(\tau')\rangle = -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta H}\mathrm{T} D_H^\dagger(\tau) D_H(\tau')\right] \ , \tag{80}$$

where $D_H(\tau) = e^{\tau H} D e^{-\tau H}$. $\mathcal{G}$ is periodic with period β ($\mathcal{G}(\tau+\beta) = \mathcal{G}(\tau)$), hence we are interested in its Fourier coefficients

$$\mathcal{G}_n = \int\limits_0^\beta d\tau e^{i\omega_n \tau}\mathcal{G}(\tau) \ , \tag{81}$$

where $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies [1]. $G^R(\omega)$ and $\mathcal{G}_n$ are related by an analytic continuation since their Lehmann representations are determined by the same weight function $\rho(\omega)$. Defining

$$\begin{aligned}
\Gamma(z) &= \int d\omega \frac{\rho(\omega)}{z-\omega} \ , \\
\rho(\omega) &= \frac{1}{Z}\left(1-e^{-\beta\omega}\right)\sum_{mn} \mid \langle n \mid D \mid m\rangle \mid^2 e^{-\beta E_m}\delta(\omega - E_n + E_m) \ ,
\end{aligned} \tag{82}$$

it is easily verified that

$$G^R(\omega) = \Gamma(\omega + i\eta) \ , \qquad \mathcal{G}_n = \Gamma(i\omega_n) \tag{83}$$

as $\eta \to 0^+$. We can therefore calculate $G^R(\omega)$ by obtaining an expression for $\mathcal{G}_n$ with an explicit dependence on $i\omega_n$, then perform the analytic continuation by formally replacing $i\omega_n \to \omega + i\eta$. We can then calculate the strength function $G(\omega)$ from (79). In general, an analytic continuation of $\mathcal{G}_n$ is not unique since it is based on extrapolating from a discrete set of points $i\omega_n$ to a continuum ω. The sum rule $\int_{-\infty}^{\infty} d\omega\rho(\omega) = \langle D^\dagger D\rangle$, however, selects a continuation that satisfies $\Gamma(z) \sim \langle D^\dagger D\rangle/z$ as $z \to \infty$ which is unique [1,2]. In this Section we present an auxiliary-field path integral treatment of $\mathcal{G}(i\omega_n) \equiv \mathcal{G}_n$ from which we extract several approximations for $G(\omega)$.

B. Strength Function in the PSPA

In the auxiliary-field path integral representation Eqs. (80) and (81) can be written in the form

$$\mathcal{G}(i\omega_n) = \frac{\int d\sigma_0 e^{-\beta F_0} \mathcal{G}_0(i\omega_n)}{\int d\sigma_0 e^{-\beta F_0}} \;, \tag{84}$$

where

$$\mathcal{G}_0(i\omega_n) = \frac{1}{\zeta_0'} \int \mathcal{D}'[\sigma] \exp\left(-\chi\beta \sum_{r>0} \mid \sigma_r \mid^2\right) \times \int_0^\beta d\tau e^{i\omega_n\tau} \langle \mathrm{T}\mathcal{U}_\sigma D^\dagger(\tau) D(0)\rangle_0 \;. \tag{85}$$

The time-dependence in D is understood to be in the interaction picture with respect to h_0, $D(\tau) = e^{\tau h_0} D e^{-\tau h_0}$. Our aim is to calculate $\mathcal{G}_0(i\omega_n)$. The connected diagrams factor out as in (51) [1,2]:

$$\begin{aligned}
&\int_0^\beta d\tau e^{i\omega_n\tau} \langle \mathrm{T}\mathcal{U}_\sigma D^\dagger(\tau) D(0)\rangle_0 = \langle \mathcal{U}_\sigma\rangle_0 \int_0^\beta d\tau e^{i\omega_n\tau} \left[\langle \mathrm{T}\mathcal{U}_\sigma D^\dagger(\tau) D(0)\rangle_c + \langle \mathrm{T}\mathcal{U}_\sigma D^\dagger(\tau)\rangle_c \langle \mathcal{U}_\sigma D(0)\rangle_c \right] \\
&= \langle \mathcal{U}_\sigma\rangle_0 \int_0^\beta d\tau e^{i\omega_n\tau} \langle D^\dagger(\tau) D(0)\rangle_c + \frac{1}{2} \langle \mathcal{U}_\sigma\rangle_0 \sum_{rs\neq 0} \sigma_r\sigma_s \int_0^\beta d\tau d\tau' d\tau'' e^{i\omega_n\tau} e^{i\omega_r\tau} e^{i\omega_s\tau} \\
&\times \left[\langle \mathrm{T}V(\tau')V(\tau'')D^\dagger(\tau)D(0)\rangle_c + 2\langle \mathrm{T}V(\tau')D^\dagger(\tau)\rangle_c \langle \mathrm{T}V(\tau'')D(0)\rangle_c \right] \;,
\end{aligned} \tag{86}$$

where terms proportional to $\delta_{n,0}$, such as

$$\int_0^\beta d\tau e^{i\omega_n\tau} \langle D^\dagger(\tau)\rangle_0 \langle D(0)\rangle_0 \;, \tag{87}$$

are omitted since they do not contribute to the analytic continuation. Similarly to (56) we can rewrite $\mathcal{G}_0(i\omega_n)$ in the form

$$\begin{aligned}
\mathcal{G}_0(i\omega_n) &= \frac{1}{\zeta_0'} \int \mathcal{D}'[\sigma] e^{-\chi\beta\sigma^T A\sigma} \left[b(i\omega_n) + \frac{1}{2} \sigma^T B(i\omega_n)\sigma \right] \\
&= b(i\omega_n) + \frac{1}{4\chi\beta} \mathrm{Tr}\left[A^{-1} B(i\omega_n) \right] \;,
\end{aligned} \tag{88}$$

where $A(\sigma_0)$ is defined in (54) and $b(\sigma_0, i\omega_n)$, $B(\sigma_0, i\omega_n)$ are given implicitly by (86). The calculation of these quantities using Wick's theorem and the frequency summation technique is similar to those discussed in previous Sections but much more cumbersome and we give here the final results. We have

$$\begin{aligned} \mathcal{G}_0^{(SPA)}(i\omega_n) &= b(\sigma_0, i\omega_n) \ , \\ \mathcal{G}_0^{(PSPA)}(i\omega_n) &= b(\sigma_0, i\omega_n) + \frac{\chi}{4\beta} \sum_{u=1}^{6} t_u(\sigma_0, i\omega_n) \ , \end{aligned} \tag{89}$$

where

$$\begin{aligned} b(\sigma_0, i\omega_n) &= -\sum_{ij} d_{ij}^\dagger d_{ji} \frac{f_i - f_j}{i\omega_n + \Delta_{ij}} \ , \\ t_1(\sigma_0, i\omega_n) &= -2 \sum_{ijkl} v_{ij} d_{ji}^\dagger v_{kl} d_{lk} \frac{f_i - f_j}{i\omega_n - \Delta_{ij}} \frac{f_k - f_l}{i\omega_n + \Delta_{kl}} \frac{\prod_{pq}' \left[(i\omega_n)^2 - \Delta_{pq}^2\right]}{\prod_\nu \left[(i\omega_n)^2 - \Omega_\nu^2\right]} \ , \\ t_2(\sigma_0, i\omega_n) &= -2 \sum_{ijkl} v_{jk} v_{kl} d_{li} d_{ij}^\dagger S_{ijkl}^{(2)} \ , \\ t_3(\sigma_0, i\omega_n) &= -2 \sum_{ijkl} v_{ij} v_{jk} d_{kl}^\dagger d_{li} S_{ijkl}^{(3)} \ , \\ t_4(\sigma_0, i\omega_n) &= -2 \sum_{ijkl} v_{ij} v_{kl} d_{ij}^\dagger d_{li} S_{ijkl}^{(4)} \ , \end{aligned} \tag{90}$$

with

$$\begin{aligned} S_{ijkl}^{(2)} &= \sum_{r \neq 0} a_r^{-1} I_{n-rr}^{ijkl} \ , \\ S_{ijkl}^{(3)} &= \sum_{r \neq 0} a_r^{-1} I_{-rrn}^{ijkl} \ , \\ S_{ijkl}^{(4)} &= \sum_{r \neq 0} a_r^{-1} I_{-rnr}^{ijkl} \ , \\ I_{tsr}^{ijkl} &= \frac{f_i}{(\Delta_{ij} + i\omega_t)(\Delta_{ik} + i\omega_{t+s})(\Delta_{il} + i\omega_{t+r+s})} \\ &\quad - \frac{f_j}{(\Delta_{ij} + i\omega_t)(\Delta_{jk} + i\omega_s)(\Delta_{jl} + i\omega_{r+s})} + \frac{f_k}{(\Delta_{ik} + i\omega_{t+s})(\Delta_{jk} + i\omega_s)(\Delta_{kl} + i\omega_r)} \\ &\quad + \frac{f_l}{(\Delta_{il} + i\omega_{t+r+s})(\Delta_{jl} + i\omega_{r+s})(\Delta_{kl} + i\omega_r)} \ . \end{aligned} \tag{91}$$

The apparent divergences of I_{ijkl}^{tsr}, e.g. when both $\Delta_{jl} = 0$ and $r + s = 0$, are handled in the usual way by taking the limit $\epsilon_j \to \epsilon_l$.

We use frequency summations to bring the infinite sums in $S_{ijkl}^{(u)}$ into closed forms:

$$S_{ijkl}^{(u)}(\sigma_0, i\omega_n) = -\sum_\alpha \frac{\beta}{e^{\beta z_\alpha} - 1} \frac{p_{ijkl}^{(u)}(z_\alpha)}{\prod_{\alpha' \neq \alpha} (z_\alpha - z_{\alpha'})} - \frac{p_{ijkl}^{(u)}(0)}{\prod_{\alpha'} (-z_{\alpha'})} \ , \tag{92}$$

where

$$
\begin{aligned}
p^{(2)}_{ijkl}(z) &= \prod_{pq}{}'(z^2-\Delta^2_{pq}) \\
&\quad \times \left[-\frac{f_i}{\eta_1\eta_2}(z-z_2)(z-z_3)+\frac{f_j}{\eta_1\eta_3}(z-z_1)(z-z_3)+f_k-\frac{f_l}{\eta_2\eta_3}(z-z_1)(z-z_2)\right] , \\
z_\alpha &= \Delta_{ik}+i\omega_n, \Delta_{jk}, -\Delta_{kl}, \pm\Omega_\nu \ , \alpha=1,2,\cdots \ , \\
\eta_1 &= \Delta_{ij}+i\omega_n, \eta_2=\Delta_{il}+i\omega_n, \eta_3=\Delta_{jl} \ ,
\end{aligned} \tag{93}
$$

$$
\begin{aligned}
p^{(3)}_{ijkl}(z) &= \prod_{pq}{}'(z^2-\Delta^2_{pq}) \\
&\quad \times \left[-\frac{f_i}{\eta_1\eta_2}(z-z_2)(z-z_3)+\frac{f_k}{\eta_1\eta_3}(z-z_1)(z-z_3)+f_j-\frac{f_l}{\eta_2\eta_3}(z-z_1)(z-z_2)\right] , \\
z_\alpha &= \Delta_{ij}, -\Delta_{jk}, -\Delta_{jl}-i\omega_n, \pm\Omega_\nu \ , \alpha=1,2,\cdots \ , \\
\eta_1 &= \Delta_{ik}, \eta_2=\Delta_{il}+i\omega_n, \eta_3=\Delta_{kl}+i\omega_n \ ,
\end{aligned} \tag{94}
$$

$$
\begin{aligned}
&p\ {}^{(4)}_{ijkl}(z) = \prod_{pq}{}'(z^2-\Delta^2_{pq}) \\
&\times \left[\frac{f_i}{\eta_1}(z-z_3)(z-z_4)+\frac{f_j}{\eta_2}(z-z_2)(z-z_4)-\frac{f_k}{\eta_2}(z-z_1)(z-z_3)-\frac{f_l}{\eta_1}(z-z_1)(z-z_2)\right] , \\
&z_\alpha = \Delta_{ij}, \Delta_{ik}+i\omega_n, -\Delta_{jl}-i\omega_n, -\Delta_{kl}, \pm\Omega_\nu \ , \alpha=1,2,\cdots \ , \\
&\eta_1 = \Delta_{il}+i\omega_n, \eta_2=\Delta_{jk}+i\omega_n \ .
\end{aligned} \tag{95}
$$

Eqs. (89)-(90) and (92)-(95) constitute our final result for $\mathcal{G}_0(i\omega_n)$. The analytic continuation (83) followed by employing the relation (79) result in

$$
G_0^{(SPA,PSPA)}(\omega) = -\frac{1}{\pi}\frac{1}{1-e^{-\beta\omega}}\mathrm{Im}\mathcal{G}_0^{(SPA,PSPA)}(i\omega_n\to\omega+i\eta) \ . \tag{96}
$$

We remark that the use of frequency summations to convert the infinite sums in $S^{(u)}_{ijkl}$ (91) into the finite expressions (92) is essential to the extraction of the strength function, since an analytic continuation of the truncated sums would result in a wrong functional form of $G(\omega)$.

The SPA expression has the simple form

$$
G_0^{(SPA)}(\omega) = \frac{1}{1-e^{-\beta\omega}}\sum_{ij} d_{ij}d^\dagger_{ji}(f_i-f_j)\delta(\omega-\Delta_{ij}) \ . \tag{97}
$$

This result illustrates a significant limitation of this approximation, namely that only transitions at frequencies ω corresponding to single-particle energy differences $\Delta_{ij}(\sigma_0)$ can be described. This shortcoming becomes evident upon performing the integration over the static field (84) which results in

$$
G^{(SPA)}(\omega) = \frac{1}{Z^{(SPA)}}\frac{1}{1-e^{-\beta\omega}}\sum_{ij}\sum_\lambda\left[e^{-\beta F_0}\frac{d_{ij}d^\dagger_{ji}(f_i-f_j)}{\mid d\Delta_{ij}/d\sigma_0\mid}\right]_{\sigma_0=\sigma_0^\lambda} \tag{98}
$$

where the second sum is over the values $\sigma_0 = \sigma_0^\lambda$ satisfying $\Delta_{ij}(\sigma_0^\lambda) = \omega$. In the case of our $U(2)$ model $\Delta_{ij} = 0, \pm 2\sqrt{\epsilon^2 + \chi^2\sigma_0^2}$, hence for $\mid \omega \mid < 2\epsilon$ the strength function $G^{(SPA)}(\omega) = 0$ and the transitions at this ω-range are not reflected.

It is interesting to compare the shell-model Monte Carlo (SMMC) methods with the PSPA. While in the SMMC the auxiliary-field path integral is evaluated exactly (except for statistical errors), the problem of extracting the strength function from the imaginary-time response function is quite difficult due to statistical noise. The strength function is calculated in the Monte Carlo using a maximal entropy reconstruction method [8,9], but this method work well only in some cases. In contrast, the PSPA strength function is extracted by exact analytic continuation (although only within the approximation). An additional advantage of the PSPA is that the infinite-discretization limit of the imaginary-time interval $[0, \beta)$ is taken exactly, whereas in the SMMC it is necessary to extrapolate the finite time step to zero. The validity of the PSPA for strength functions is tested in Sections V.C and V.D.

C. Moments of the Strength Function

The moments of the strength function

$$M_n = \int_{-\infty}^{\infty} d\omega \; \omega^n G(\omega) \; , \qquad n = 0, 1, 2, ... \tag{99}$$

provide another measure of the quality of the approximations we develop. Rather than integrating over the expressions we have for $G(\omega)$, it is more convenient to obtain the moments directly in terms of H and D. From $G(\omega)$ being the Fourier transform of $G(t)$ it follows that

$$M_n = i^n \frac{d^n G}{dt^n} \mid_{t=0} \; , \tag{100}$$

and differentiating the definition of $G(t)$ (second Eq. in (74)) we get for the lowest moments

$$\begin{aligned} M_0 &= \langle D^\dagger D \rangle \; , \\ M_1 &= \frac{1}{2} \langle \left[D^\dagger, [H, D] \right] \rangle \; . \end{aligned} \tag{101}$$

Thus the zeroth moment (total strength) is simply a two-body expectation value, which was discussed in the previous Section and found to be well reproduced by the PSPA (contrary to the SPA) in our $U(2)$ model (see Fig. 4).

The first moment M_1 (M_1/M_0 is average transition energy) is also given by the expectation value of a two-body operator. Taking $D = J_x$ in our $U(2)$ model we can exploit the angular-momentum commutation relations to get $M_1 = 2i\epsilon\langle J_x J_y \rangle$. The latter is calculated by a generalization of the results for $\langle D^\dagger D \rangle$ obtained in the previous Section to the case $\langle D_1^\dagger D_2 \rangle$: whereas d_{ij} in (90) is the matrix corresponding to D_2, $d_{ij}^\dagger$ should be taken to be that of $D_1^\dagger$. The results for M_1 are shown in Fig. 6 for different values of the mean-field

parameter κ in (47). The PSPA agrees well with the exact result. The SPA is good at high temperatures but worsens appreciably near the mean-field transition and below it, except for the no-transition case ($\kappa = 0.5$) where it remains a good approximation also at low temperatures. This comparison is interesting in view of the results of Ref. [16] where two versions of the static approximation for the strength function were tested. The first version (called the adiabatic approximation) is identical to our SPA. The second version (called the static-path approximation in Ref. [16]) consists of estimating the path integral representation of $\mathcal{G}(\tau)$ in (80) by step function paths $\xi(\tau')$ which have a discontinuity at $\tau' = \tau$,

$$\xi(\tau') = \left\{ \begin{array}{ll} \sigma_0 \,, & 0 \le \tau' < \tau \\ \rho_0 \,, & \tau \le \tau' < \beta \end{array} \right\} \tag{102}$$

rather than by the constant ones ($\sigma_0 = \rho_0$) alone. We shall discuss this approximation further below. The PSPA includes the effect of discontinuous paths only to the second order in $\sigma_0 - \rho_0$ through the correction factor from small oscillations about the average value $\sigma_0 \tau/\beta + (\rho_0 - \sigma_0)(1 - \tau/\beta)$. It was found in Ref. [16] that although the inclusion of the discontinuous paths (102) provided an improvement over the SPA, a good agreement with the exact results was not achieved, contrary to the situation in the PSPA case. This suggests that the important contribution to the moments of the strength function beyond the SPA comes from small-amplitude oscillatory paths rather than from step function paths with a large discontinuity.

D. Strength Function in a Simple Model: Results and Discussion

We test the PSPA for $G(\omega)$ in our $U(2)$ model with perturbing operators $D = J_x$ and $D = J_y$. The results are presented in Fig. 7 and Fig. 8, respectively. We consider the same three cases studied previously characterized by $\kappa = 0.5, 1.5, 3.0$ at different temperatures, chosen to be at the mean-field transition in each case as well as above and below it (a transition does not occur for $\kappa = 0.5$). Note that the exact result (B9) consists of a sum of δ-functions in the limit $\eta \to 0^+$ and is therefore singular, as is the case for the MFA result. This is not the situation in the SPA and PSPA which involve an integration over the static field σ_0. In order to facilitate a meaningful comparison we keep η small but finite both in the exact result, which becomes a sum of Lorentzians of width η, and in the approximations. Finally, we plot $G(\omega)$ only for positive ω since $G(-\omega) = e^{-\beta\omega} G(\omega)$ for an Hermitean D.

The shortcoming of the SPA expressions (97)-(98) is manifested clearly in Figs. 7 and 8. Since we use $\epsilon = 1$ the SPA strength function cannot reflect transitions with $\omega < 2$. Hence it vanishes in the range $\omega < 2$ even if most of the strength is concentrated there, as is the case for $\kappa = 0.5, 1.5$ at $\beta = 1.7, 3.0$ (where the SPA result has a shifted peak near $\omega = 2$ to the right of the exact peak). Furthermore, since the PSPA result consists of an additive correction to the SPA expression (see Eq.(89)), this shifted SPA peak leaves its trace in the PSPA strength function. For $\kappa = 0.5$, for instance, even though the main PSPA peak is in excellent agreement with the exact one, it is accompanies by a small additional (false) peak to its right, left over from the SPA, which becomes larger as the temperature decreases. In general, the PSPA works quite well for small κ but decreases in quality and becomes comparable with the SPA as κ increases or the temperature decreases. The MFA generates

a sharp peak located near the middle of the broader SPA peak, consistently with its origin as a steepest-descent approximation of the SPA integral.

We mentioned above that in Ref. [16] $G(\omega)$ was calculated in a modified static-path approach which included constant paths with a discontinuity at τ in the path integral representation of $\mathcal{G}(\tau)$. It is interesting to note that the resulting strength function in [16] is accurate for large values of κ and deteriorates as κ decreases, in contrast with the PSPA result. This suggests that for small κ the major contribution to the strength function beyond static fields comes from small oscillations about them. However, for large κ these small oscillations are negligible and large imaginary-time discontinuities in the static fields become important. It is therefore desirable to have an approximation scheme which takes both contributions into account. In the following we discuss an approach to this problem in the imaginary-time framework and the difficulties it encounters.

We start from the auxiliary-field path integral representation of the imaginary-time response function

$$\mathcal{G}(\tau) = -\frac{1}{Z}\mathrm{Tr}\left[e^{-(\beta-\tau)H}D^\dagger e^{-\tau H}D\right] = -\frac{1}{Z}\int \mathcal{D}[\xi]\exp\left[-\frac{1}{2}\chi\int_0^\beta d\tau\xi^2(\tau)\right]$$
$$\times\ \mathrm{Tr}\left\{\mathrm{T}\exp\left[-\int_\tau^\beta d\tau'\left(K-\xi(\tau')V\right)\right]D^\dagger\mathrm{T}\exp\left[-\int_0^\tau d\tau'\left(K-\xi(\tau')V\right)\right]D\right\}\ . \tag{103}$$

However, rather than use the Fourier decomposition (10) of $\xi(\tau')$ over the entire interval $[0,\beta)$ to obtain the form (84), (85) from which the SPA and PSPA are derived, we divide the intervals $[0,\tau)$ and $[\tau,\beta)$ into N and M sub-intervals, respectively, and use separate decompositions in each. We have

$$\xi(\tau') = \left\{\begin{array}{ll}\sum\limits_{r=-(N-1)/2}^{(N-1)/2}\sigma_r e^{i\omega_r\tau'}\ , & 0\le\tau'<\tau\\ \sum\limits_{r=-(M-1)/2}^{(M-1)/2}\rho_r e^{i\nu_r\tau'}\ , & \tau\le\tau'<\beta\end{array}\right\}\ , \tag{104}$$

with the reality condition $\sigma_{-r}=\sigma_r^*$, $\rho_{-r}=\rho_r^*$ and τ-dependent frequencies $\omega_r=2\pi r/\tau$, $\nu_r = 2\pi r/(\beta-\tau)$. In terms of the new variables the representation (103) becomes

$$\mathcal{G}(\tau) = -\frac{1}{Z}\int\mathcal{D}[\sigma]\mathcal{D}[\rho]\exp\left[-\frac{1}{2}\chi\tau\sum_r\mid\sigma_r\mid^2-\frac{1}{2}\chi(\beta-\tau)\sum_r\mid\rho_r\mid^2\right]$$
$$\times\ \mathrm{Tr}\left\{\mathrm{T}\exp\left[-\int_\tau^\beta d\tau'\left(K-\chi\sigma_0V-\chi\sum_{r\neq0}\sigma_r e^{i\omega_r\tau'}V\right)\right]D^\dagger\right.$$
$$\left.\times\ \mathrm{T}\exp\left[-\int_0^\tau d\tau'\left(K-\chi\rho_0V-\chi\sum_{r\neq0}\rho_r e^{i\nu_r\tau'}V\right)\right]D\right\}\ . \tag{105}$$

The discontinuous static-path approximation (DSPA), originally introduced in [16] using the real-time framework, is now obtained by neglecting the contribution of the oscillations about the static paths (102) which results in the two-dimensional integral

$$\mathcal{G}^{(DSPA)}(\tau) = -\frac{1}{Z^{(DSPA)}}\frac{\chi}{2\pi}\sqrt{\beta(\beta-\tau)}\int d\sigma_0 d\rho_0 e^{-\frac{1}{2}\chi\left[\tau\sigma_0^2+(\beta-\tau)\rho_0^2\right]}$$
$$\times \mathrm{Tr}\left[e^{-(\beta-\tau)(K-\chi\rho_0 V)}D^\dagger e^{-\tau(K-\chi\sigma_0 V)}D\right] \ . \tag{106}$$

The partition function in this approximation in given by

$$Z^{(DSPA)} = \frac{\chi}{2\pi}\sqrt{\beta(\beta-\tau)}\int d\sigma_0 d\rho_0 e^{-\frac{1}{2}\chi\left[\tau\sigma_0^2+(\beta-\tau)\rho_0^2\right]}\mathrm{Tr}\left[e^{-(\beta-\tau)(K-\chi\rho_0 V)}e^{-\tau(K-\chi\sigma_0 V)}\right] \ . \tag{107}$$

Note that $Z^{(DSPA)}$ acquires a τ-dependence.

In order to carry out the imaginary-time technique of Fourier-transforming $\mathcal{G}(\tau)$ to get $\mathcal{G}(i\omega_n)$ and extract the strength function $G(\omega)$ by an analytic continuation as was done above, it is necessary to obtain the functional dependence on τ in (106) analytically. However, the τ-dependence of the traces involved is non-trivial and had to be studied numerically in Ref. [16] even for the simple $U(2)$ model; note that the analogous situation in the real-time framework (namely that the t-dependence of $G^{(DSPA)}(t)$ is not given analytically) does not pose a problem since a numerical Fourier transform produces $G^{(DSPA)}(\omega)$ directly. Furthermore, unlike the SPA case where we had a static Hamiltonian h_0 and Wick's theorem could be used to calculate the traces, here we have a discontinuous Hamiltonian

$$h_0(\tau') = \left\{ \begin{array}{ll} K-\chi\sigma_0 V \ , & 0 \le \tau' < \tau \\ K-\chi\rho_0 V \ , & \tau \le \tau' < \beta \end{array} \right\} \ , \tag{108}$$

for which Wick's theorem is not applicable. In particular, without a generalization of Wick's theorem to this situation, it would be difficult to use our methods to calculate corrections due to small oscillations about the discontinuous paths.

VI. CONCLUSION

In this paper we present an approximation scheme, the PSPA, for the calculation of thermodynamic quantities and finite temperature response functions in finite fermionic systems. The approximation is derived in the framework of the auxiliary-field path integral. We use an imaginary-time formulation which facilitates the extension of this approximation to physical quantities beyond the free energy and the level density to which it was previously limited.

Testing the PSPA in a simple many-body model, we find that it improves on the SPA and is a good approximation for expectation values of observables as well as for low moments of strength functions. This indicates that the contribution of time-dependent fluctuations about the static fields (neglected in the SPA) is significant. The required computational work involved in the PSPA includes a q-dimensional numerical integration over the static fields σ_0^α and a diagonalization of a $q\times q$ matrix at each σ_0^α-point, where q is the number of separable interactions in the Hamiltonian. This approximation breaks down at low temperatures when the small-oscillation correction factor diverges for the dominant static fields, indicating that large time-dependent fluctuations become important. However, the breakdown occurs at temperatures well below the mean-field transition and does not affect the usefulness of the PSPA except at very low temperatures. For the strength function itself the PSPA results

become less reliable when the contribution of static paths with large discontinuity (at the time where the response function is calculated) is important. Further improvement would require the inclusion of both discontinuous static paths and small time-dependent oscillations around them.

It would be interesting to test the PSPA methods for more realistic nuclear interactions, such as pairing plus multipole interactions. For these interactions, the SPA works better in a mixed pairing-density decomposition than in a pure density decomposition. Thus, it would be useful to extend the present PSPA techniques to such a mixed pairing-density decomposition in the HS representation.

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APPENDIX: RPA FREQUENCIES AT FINITE TEMPERATURE

The finite temperature RPA equations for a general two-body interaction u_{ijkl} are given by [3]

$$-\Delta_{ij}\xi^{\nu}_{ij} + \sum_{k,l} u_{iljk}(f_k - f_l)\xi^{\nu}_{kl} = \Omega_\nu \xi^{\nu}_{ij} \;, \tag{A1}$$

where $\Delta_{ij} = \epsilon_i - \epsilon_j$ and f_i are the Fermi-Dirac occupation numbers $f_i = (1 + e^{\beta\epsilon_i})^{-1}$. The solutions of (A1) are the RPA frequencies Ω_ν and ξ^ν are the associated RPA amplitudes. The single-particle energies ϵ_i in (A1) correspond to the mean-field solution $\bar{\sigma}_0$ but in the following we replace $\bar{\sigma}_0$ by a general static field σ_0.

For a separable interaction as in (1) with V Hermitean, or more generally for an interaction as in (3) which is a sum of q such separable terms, $u_{iljk} = -\sum_\alpha \chi_\alpha v^\alpha_{ij} v^\alpha_{lk}$, and Eq. (A1) can be rewritten as

$$\xi^\nu_{ij} = -\sum_\alpha \chi_\alpha \frac{v^\alpha_{ij}}{\Delta_{ij} + \Omega_\nu}\left[\sum_{kl} v^\alpha_{lk}(f_k - f_l)\xi^\nu_{kl}\right] \;. \tag{A2}$$

(A2) can be converted to a set of coupled equations for the q quantities

$$\zeta^\nu_\alpha \equiv \sum_{kl} v^\alpha_{lk}(f_k - f_l)\xi^\nu_{kl} \tag{A3}$$

by multiplying Eq. (A3) by $v^{\alpha'}_{ji}(f_i - f_j)$ and summing over ij for each $\alpha' = 1, \ldots, q$. We get

$$\sum_\alpha \left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v^{\alpha'}_{ji} v^\alpha_{ij} \frac{f_i - f_j}{\Delta_{ij} + \Omega_\nu}\right]\zeta^\nu_\alpha = 0 \;; \quad \alpha' = 1, \ldots, q \;. \tag{A4}$$

For (A4) to have a non-trivial solution (i.e. not all $\zeta^\nu_\alpha = 0$), we require that the determinant of the coefficient matrix vanishes

$$\det\left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v^{\alpha'}_{ji} v^\alpha_{ij} \frac{f_i - f_j}{\Delta_{ij} + \Omega_\nu}\right] = 0 \;. \tag{A5}$$

Regarding the l.h.s. of Eq. (A5) as a function of ω, where we have substituted ω for Ω_ν, we notice that its roots are $\pm\Omega_\nu$, while its poles are $\pm\Delta_{ij}$. It then follows that

$$\det\left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v_{ji}^{\alpha'} v_{ij}^{\alpha} \frac{f_i - f_j}{\Delta_{ij} + \omega}\right] = \frac{\prod_\nu (\Omega_\nu^2 - \omega^2)}{\prod_{ij}{}'(\Delta_{ij}^2 - \omega^2)} \; . \tag{A6}$$

Upon the substitution $\omega \to i\omega$ we find

$$\det\left[\delta_{\alpha'\alpha} + \chi_\alpha \sum_{ij} v_{ji}^{\alpha'} v_{ij}^{\alpha} \frac{f_i - f_j}{\Delta_{ij} + i\omega}\right] = \frac{\prod_\nu (\Omega_\nu^2 + \omega^2)}{\prod_{ij}{}'(\Delta_{ij}^2 + \omega^2)} \; . \tag{A7}$$

Using Eq. (A7) for $\omega = \omega_r$ one obtains (36) or (41) when one or several separable terms in the interaction are present, respectively.

APPENDIX: THE MODEL

The formalism developed in this paper is illustrated and tested in a simple Fermionic system, a variant of a model introduced in [25] which is based on a $U(2)$ algebra and is therefore solvable. This is a two-level system where each level is g-fold degenerate and may therefore contain between zero and $2g$ Fermions. The Hamiltonian is given in terms of quasi-angular momentum operators

$$H = 2\epsilon J_z - 2\chi J_x^2 \tag{B1}$$

which has the form (1) with $K = 2\epsilon J_z$ and $V = 2J_x$. The quasi-angular momentum operators are given by

$$\begin{aligned} J_x &= \frac{1}{2}\sum_{i=1}^{g}\left(a_{1i}^\dagger a_{2i} + a_{2i}^\dagger a_{1i}\right) \; , \qquad J_y = -\frac{i}{2}\sum_{i=1}^{g}\left(a_{1i}^\dagger a_{2i} - a_{2i}^\dagger a_{1i}\right) \; , \\ J_z &= \frac{1}{2}\sum_{i=1}^{g}\left(a_{1i}^\dagger a_{1i} - a_{2i}^\dagger a_{2i}\right) \; , \qquad \hat{N} = \sum_{i=1}^{g}\left(a_{1i}^\dagger a_{1i} + a_{2i}^\dagger a_{2i}\right) \end{aligned} \tag{B2}$$

with $\hat{N}$ being the particle-number operator. The 2^{2g} states are arranged in $U(2)$-multiplets (n,j) where the quantum numbers are the number of particles $n = 0, ..., 2g$ and the quasi-angular momentum $j = 0, ..., n/2$ or $1/2, ..., n/2$ (depending on whether n is even or odd). Each multiplet (n,j) contains $2j+1$ states labeled by $\mid njm\rangle$ with $m = -j, ..., j$ are the eigenvalues of J_z. To find the number $d_n(j)$ of (n,j)-multiplets we first observe that the number of states with given n and m is

$$\mathcal{N}_n(m) = \binom{g}{n/2 - m}\binom{g}{n/2 + m} \; . \tag{B3}$$

Since every multiplet (n,j') with $j' \geq j$ contributes a single state with $J_z = j$, we also have

$$\mathcal{N}_n(j) = \sum_{j'=j}^{n/2} d_n(j') \; . \tag{B4}$$

Therefore

$$\begin{aligned} d_n(j) &= \mathcal{N}_n(j) - \mathcal{N}_n(j+1) \\ &= \binom{g}{n/2-j}\binom{g}{n/2+j} - \binom{g}{n/2-j-1}\binom{g}{n/2+j+1} \; , \end{aligned} \tag{B5}$$

which checks to give

$$\sum_{j=0(1/2)}^{n/2} (2j+1) d_n(j) = \binom{2g}{n} \; , \tag{B6}$$

the total number of states with n particles.

The Hamiltonian matrix in this basis is block-diagonal with $d_n(j)$ identical blocks of dimension $2j+1$ for each pair (n, j), whose diagonalization gives the energies E_{jm} and corresponding eigenstates. The exact partition function in the grand canonical ensemble is then

$$Z = \sum_{n=0}^{2g} \sum_{j=0(1/2)}^{n/2} d_n(j) \sum_{m=-j}^{j} e^{-\beta(E_{jm}-\mu n)} \; . \tag{B7}$$

The expectation value of an operator O is given by

$$\langle O \rangle = \frac{1}{Z} \sum_{n=0}^{2g} \sum_{j=0(1/2)}^{n/2} d_n(j) \sum_{m=-j}^{j} \langle jm \mid O \mid jm \rangle e^{-\beta(E_{jm}-\mu n)} \; . \tag{B8}$$

The strength function associated with an operator O is given by

$$\begin{aligned} G(\omega) = \frac{1}{Z} \sum_{n=0}^{2g} \sum_{j=0(1/2)}^{n/2} d_n(j) \sum_{mm'=-j}^{j} \mid \langle jm' \mid O \mid jm \rangle \mid^2 e^{-\beta(E_{jm}-\mu n)} \\ \times \frac{1-e^{-\beta(E_{jm'}-E_{jm})}}{1-e^{-\beta\omega}} \mathrm{Im}\left[-\frac{1}{\pi}\frac{1}{\omega-(E_{jm'}-E_{jm})+i\eta}\right] \; , \end{aligned} \tag{B9}$$

which reduces to a sum over δ-functions as $\eta \to 0^+$.

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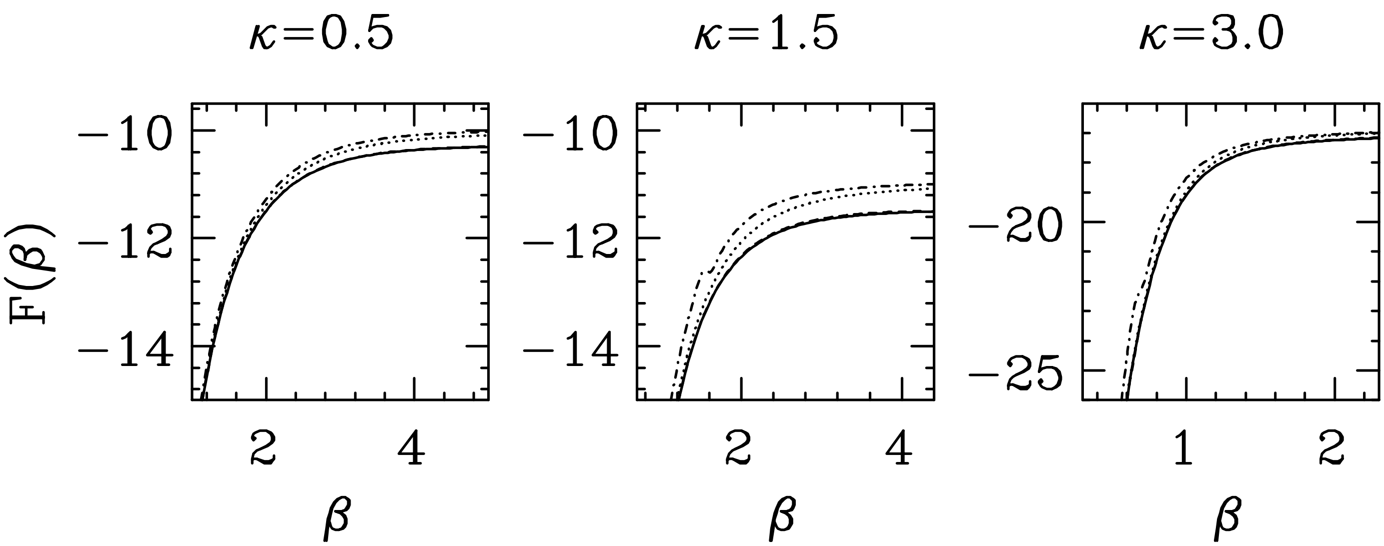

FIG. 1. Free energy $F(\beta) = -\beta^{-1}\log Z$ as a function of β for different values of κ (see (47)). The SPA (dotted) and PSPA (dashed) results are obtained using (45) in Eqs. (26) and (37). The MFA result (dashed-dotted) is given by a steepest-descent treatment of the SPA integral. The exact result (solid) is calculated from (B7).

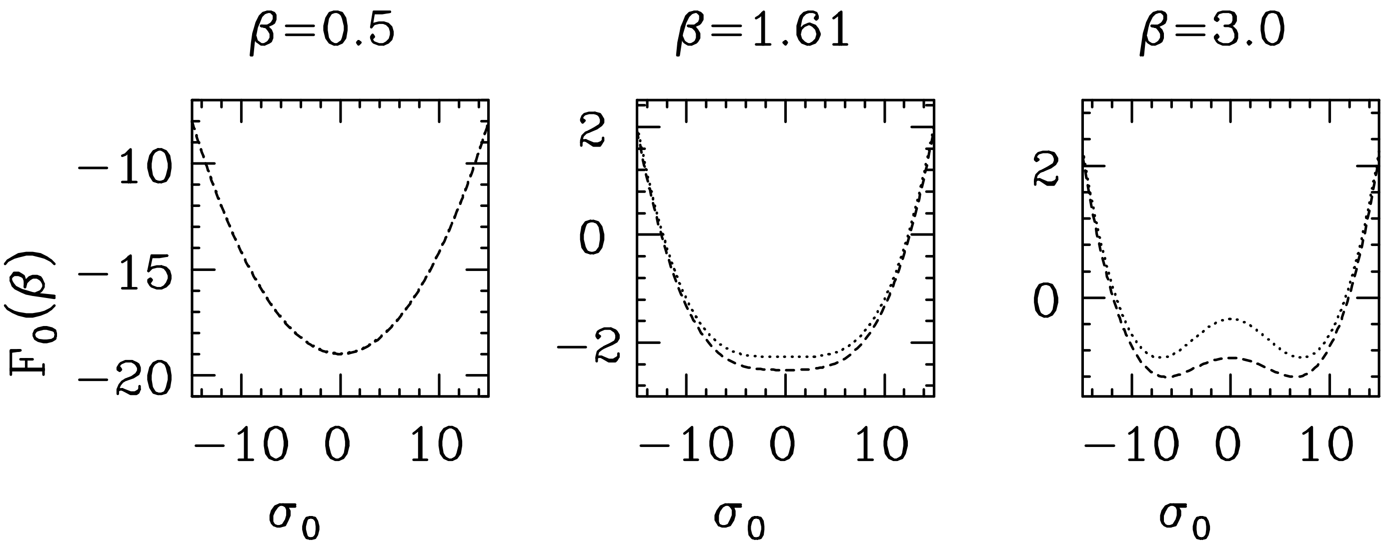

FIG. 2. Effective static-field free energy $F_0(\beta;\sigma_0)$ (24) as a function of σ_0 in the SPA (dotted) and PSPA (dashed) at different temperatures β. Shown is the case $\kappa = 1.5$ where the mean-field phase-transition occurs at $\beta_c = 1.61$.

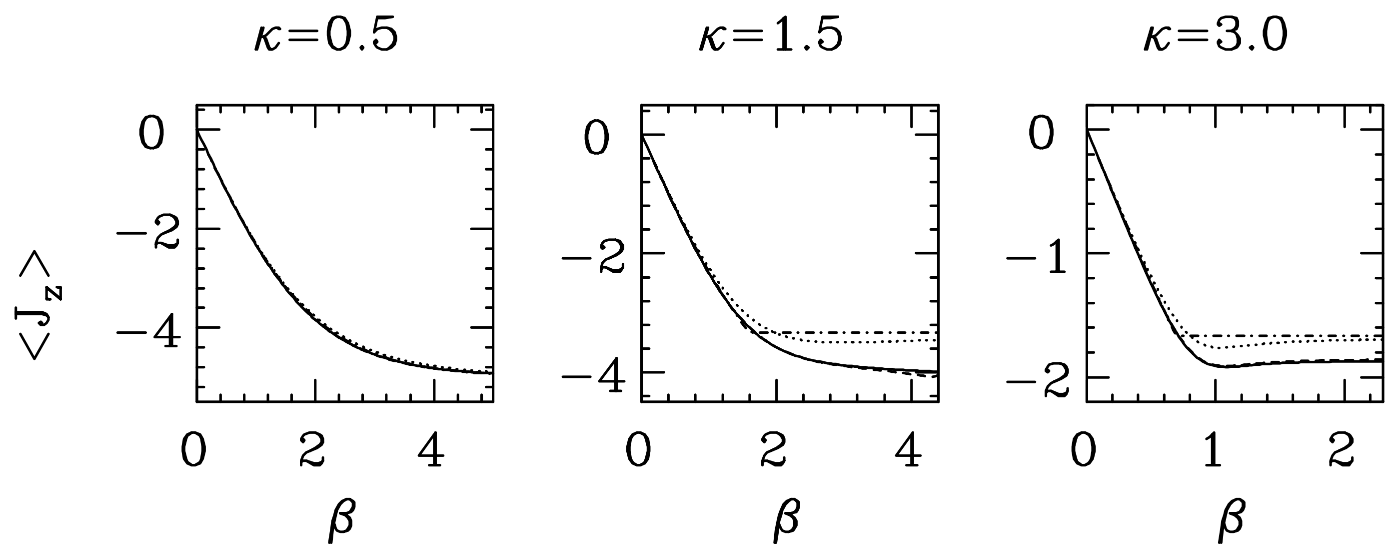

FIG. 3. Expectation value of J_z as a function of β for different values of κ. The SPA result (dotted) is given by (65) and the MFA result (dashed-dotted) is obtained from it by steepest descent. The PSPA result (dashed) is calculated using (43)-(45) and (62)- (64). These approximations are compared with the exact result (B8) (solid).

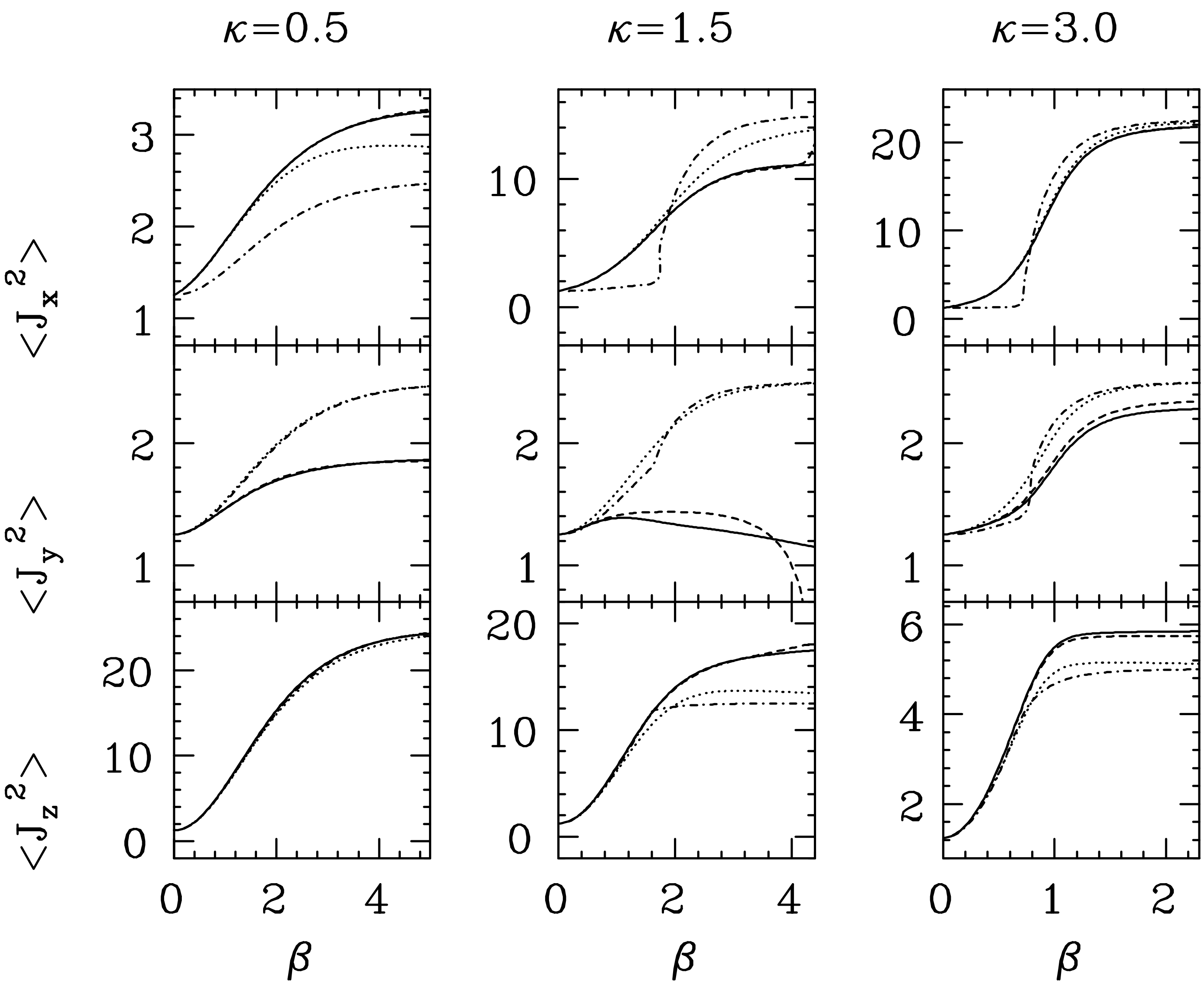

FIG. 4. Expectation value of J_x^2, J_y^2 and J_z^2 as functions of β for different values of κ. The SPA result (dotted) is given by (72) and the MFA result (dashed-dotted) is obtained from it by steepest descent. The PSPA result (dashed) is calculated using (43)-(45) and (68)-(71). These approximations are compared with the exact result (B8) (solid).

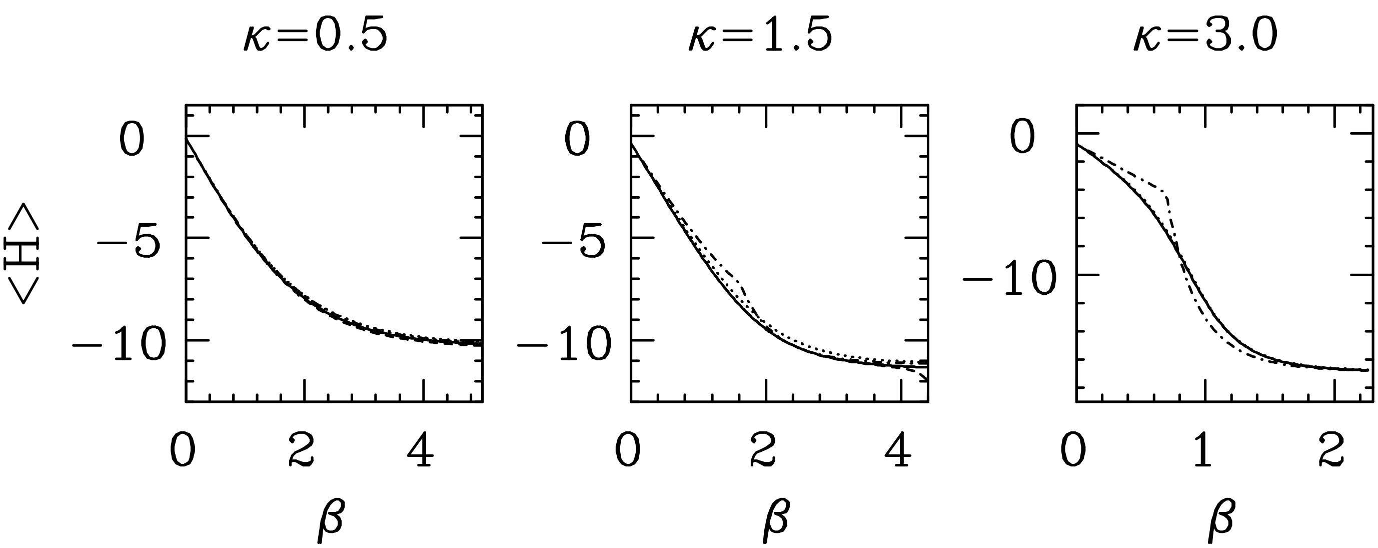

FIG. 5. Expectation value of the Hamiltonian $H = 2\epsilon J_z - 2\chi J_x^2$ (B1) as a function of β for different values of κ. Shown are the SPA (dotted), MFA (dashed-dotted), PSPA (dashed) and exact (solid) results.

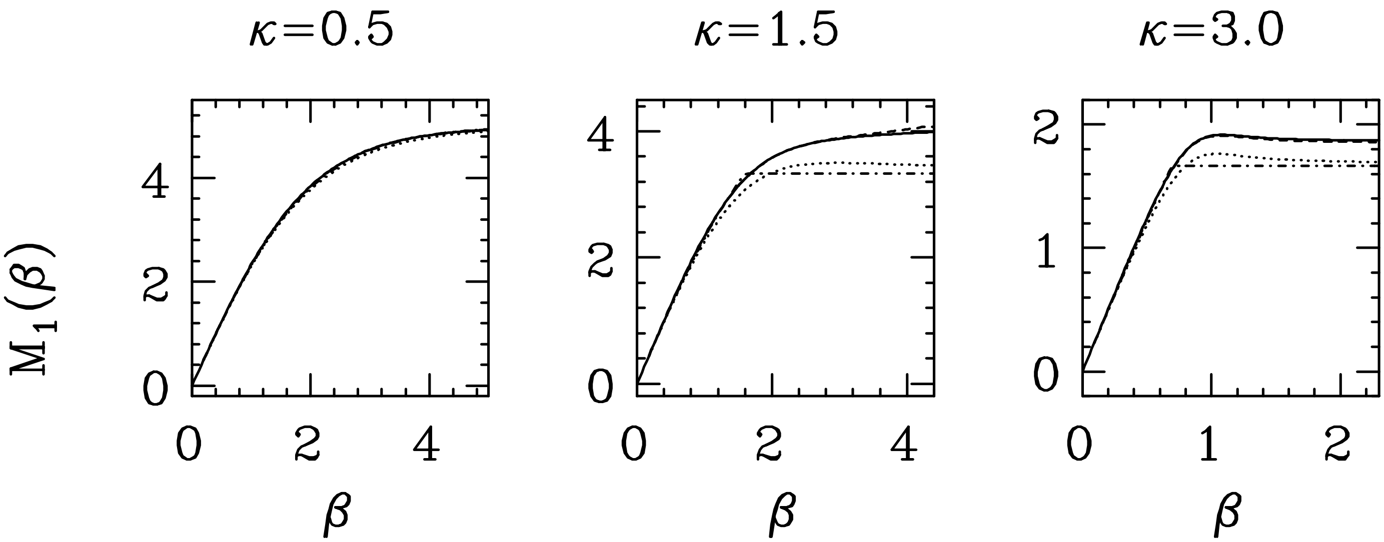

FIG. 6. First moment of the strength function $M_1 = \int_{-\infty}^{\infty} d\omega\ \omega G(\omega)$ as a function of β for different values of κ, using (101) with $D = J_x$. Shown are the SPA (dotted), MFA (dashed-dotted), PSPA (dashed) and exact (solid) results.

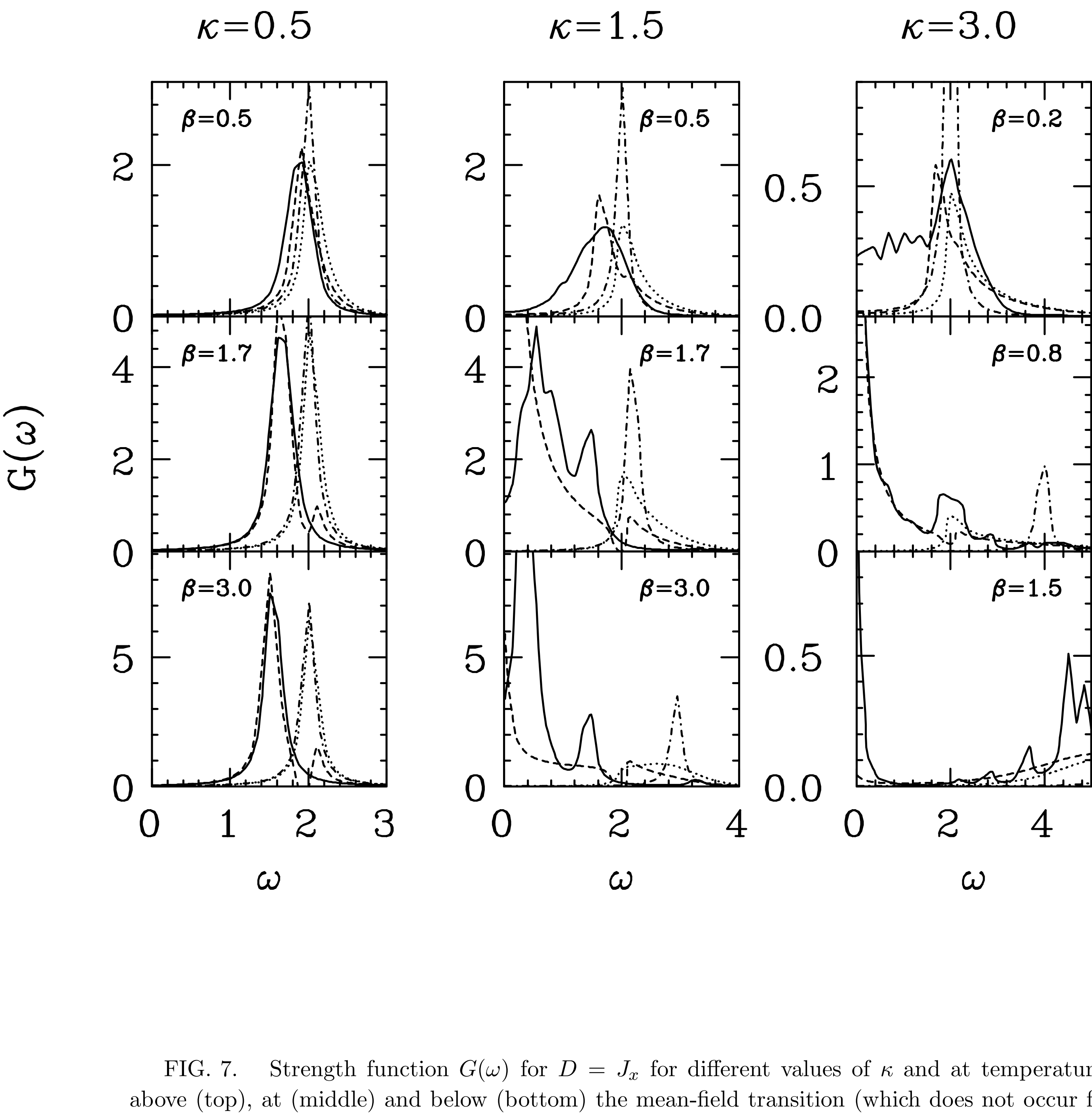

FIG. 7. Strength function $G(\omega)$ for $D = J_x$ for different values of κ and at temperatures above (top), at (middle) and below (bottom) the mean-field transition (which does not occur for $\kappa = 0.5$). Results are obtained using (89)-(90) and (92)-(96) with $\eta = 0.1$. Shown are the SPA (dotted), MFA (dashed-dotted), PSPA (dashed) and exact (B9) (solid) results.

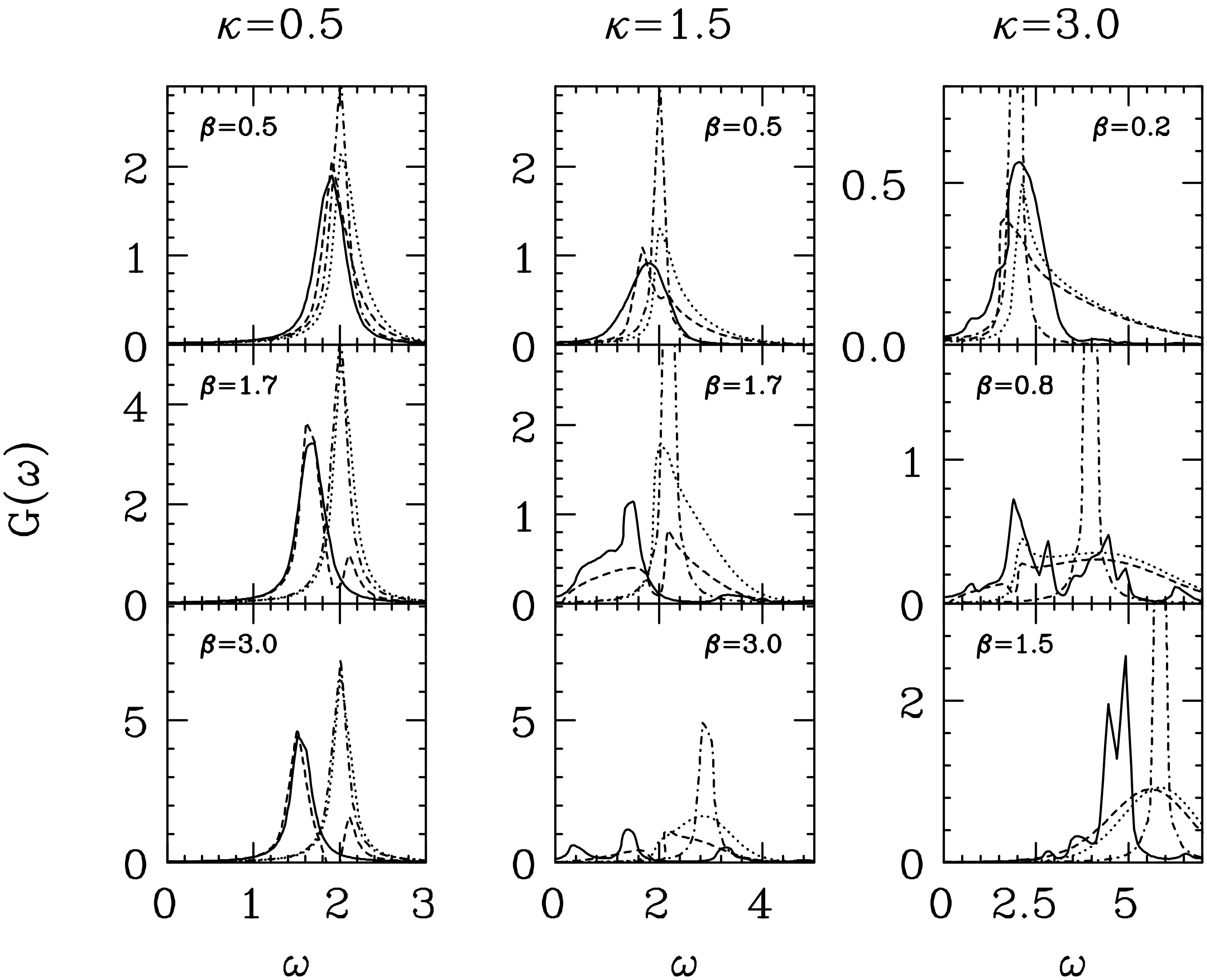

FIG. 8. Same as in Fig. 7 but for $D = J_y$.